Dictionary of Alkaloids

SECOND EDITION

with CD-ROM

EDITED BY

John Buckingham
Keith H. Baggaley
Andrew D. Roberts
László F. Szabó

CRC Press
Taylor & Francis Group

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Dictionary Entries

Foreword

Plants containing alkaloids have served humankind since ancient times. Indeed, some of the oldest surviving written records of commercial transactions involving medicinal plants are of alkaloid-containing plants. For thousands of years, indigenous groups around the world discovered, through self-experimentation with locally available plant extracts, that they could provide materials for hunting prey, culinary enhancement, amelioration from disease, relief of pain, and healing. These plants contributed significantly to the survival of indigenous groups throughout history. This same process of low-throughput clinical screening also identified many plants which were to be avoided because of their toxicity, again due to alkaloids. It is the oral and written records of these investigations which survive today and form the basis of both clinical care in much of the world and aspects of contemporary drug discovery.

A transition occurred at the beginning of the 19th century when investigations on the most significant medicinal and toxic plants of Europe commenced, these included studies on opium, colchicum, nux vomica, ipecac, belladonna, and pepper. As it transpired, all of the isolated, biologically active compounds were alkaloids, and it was these investigations which initiated the diverse studies of alkaloids as a class of natural products which continue today.

Since those early times, there have been six important phases to the study of alkaloids. The first was the tremendous increase in the number of structurally unique and complex alkaloids isolated from plants, structures which defined the new field of heterocyclic chemistry. The second was the dramatic reduction in time and the amount of material required to determine the precise stereochemical and conformational structure of an individual alkaloid as a result of the advances in spectroscopic and chromatographic techniques which permitted ever smaller samples to be structurally characterized. Third, there evolved the understanding that groups of structurally similar alkaloids could, sometimes, be related to each other based on one or two biosynthetic precursors from which chemically rational metabolic schemes could be used to generate the plethora of alkaloid skeleta and structures. Fourth, there was the recognition that this structural diversity, skeletal complexity, and stereo-uniqueness were at the same time a benefit and a bane. While the activity could be exquisite, alkaloids may also have significantly modulated biological activity based on a transformation at a single functional group or stereochemical center. Fifth, as more complex alkaloids were structurally elucidated they became challenging targets for synthetic organic chemists, and continue to be the basis for the stimulation of numerous brilliant synthetic strategies and innovations in organic chemistry. Finally, as knowledge of the biology associated with alkaloids grew in both breadth and depth, initially at the *in vivo* level and eventually at the molecular level, some alkaloids were established to be archetypal entity for a particular biological response.

Consequently, in this 200-year period, many alkaloids became critical components of the global pharmaceutical armamentarium, and tremendous healing has resulted from their clinical application. As our food and beverage practices have evolved, alkaloids have become a core component of every day life for almost everyone on the planet on a moment to moment basis, and caffeine, capsaicin, nicotine, theobromine, adrenaline, dopamine, serotonin, etc. are representative examples. Many of the colors of flowers and vegetables are due to alkaloids, and at the same time, alkaloids represent enormous and potent biological power. Sometimes this power can be ameliorated by dose reduction to produce health beneficent agents (for example, the ergot alkaloids and aconitine); in other instances they must simply be avoided by both animals and humans, such as those in many toxic plants, animals, and fungi. Alkaloids also have led medicinal chemists down productive pathways for drug development, although it is seldom appreciated that the molecular phylogeny of many synthetic drugs can be traced to classical alkaloids such as morphine and atropine. At the same time, there is a ‘‘dark side’’ to alkaloids, because at least three - morphine, cocaine, and nicotine - have powerful social implications causing tremendous human suffering through addiction, disease development, and wars which continue unabated today. It is this good, bad, and downright ugly aspect to alkaloids which has fascinated so many scientists for so long. As a global society we do indeed have this love-hate relationship with alkaloids unlike that of any other group of natural products.

As mentioned, with the rise of spectroscopy beginning in the 1950s, interest developed in examining alkaloids from wider sources than higher plants. Indeed, it appears now that almost every class of organism, insects, reptiles, birds, fungi, bacteria, the diversity of marine organisms, and mammals, including humans, all produce alkaloids. The last twenty years have witnessed an explosion in the numbers and the structural diversity of alkaloids from these sources, and these developments are dramatically reflected in this updated compilation.

From a chemical perspective, it transpires that there is almost no overlap in the structural diversity of plant, fungal, and marine alkaloids. Each is a chemically brilliant world unto itself. Thus, one would not expect to find a monoterpenoid indole alkaloid in a marine sponge, nor a manzamine alkaloid in a tropical liana. This unimaginable structural diversity places the alkaloid sciences on the cusp of a deeper understanding of their biosynthetic formation. While significant and successful efforts are underway to elucidate pathways and isolate genes which are related to both plant and fungal alkaloids, for marine organisms this aspect is completely unexplored, although the most spectacular new skeleta and potent biological activities are derived from these marine sources.

The past twenty years have witnessed the evolution of three new areas of alkaloid chemistry and biology. The first is that of the integrity of alkaloid biosynthesis. Alkaloids such the ansa macrolides from *Maytenus* and from *Colubrina*, as well as the ergot alkaloids of the Convolvulaceae are now established to be derived biosynthetically from parasitic or symbiotic fungal organisms, not through the metabolic pathways of the host plant. Second, structural conclusions regarding individual alkaloids can change; an α-hydroxy group of yesterday can become a β-hydroxy today based on refined chemical, spectroscopic, and crystallographic conclusions. As one looks through the *Dictionary of Alkaloids*, it is important to be aware that there are many examples where the synthesis of a proposed structure has failed to support that structure, or where new spectroscopic evidence does not support a proposed structure. While in some cases this has led to refinement of the structure, in others a dangling question remains as to the true identity of the natural alkaloid. Third, there is the connection of alkaloids to the biotechnology revolution, and the marvelous progress that has been made for certain alkaloid pathways in elucidating the enzymes and genes of alkaloid biosynthesis.

What, then, is the "fit" for the *Dictionary of Alkaloids,* and why is it such an important resource for researchers? Burgeoning efforts at structure elucidation and biological experimentation make it extremely difficult to quickly find key literature citations to original sources of information on individual compounds. It was recognized some years ago that there was a core global need for information systems on the isolation, spectral properties, and biological properties of alkaloids. The *Dictionary of Alkaloids* is a critical, absolutely essential component in filling that need. It is the only accumulation in the world of the taxonomy, chemistry, and biology of alkaloids derived from all sources. It provides extensive information to references for the isolation, spectroscopy, and biology of an individual alkaloid, and to its other attributes and uses. Importantly, the alkaloids are frequently collected as a group based on a parent structure. This simplifies the presentation, and accumulates alkaloids having quite different trivial names. The volume is easy to use, and the diverse indexes place the most significant information at one's fingertips. It is a unique resource, and one which is indispensable to any alkaloid chemist and biologist. The inclusion of a fully substructure searchable CD-ROM in this second edition makes the resource even more valuable.

In spite of the vast range of studies of alkaloids over the years, much remains to be done. There are many plant families which are known to contain alkaloids where the alkaloids remain to be identified; there are untold marine organisms and tens of thousands of microorganisms with unknown alkaloids. There is the genetics of alkaloid biosynthesis in more diverse organisms, and the tremendous potential for being able to produce alkaloids through isolated and stabilized systems in a sustainable manner. The key justification for alkaloid research, though, must be relevance to the enhancement of public health. For many years, justification for alkaloid research was based on their novelty; there was no relationship to biology. Indeed, it was shown several years ago that about 75% of all plant alkaloids had never been evaluated in a single bioassay. There remains a critical need for the wider biological study of known and new alkaloids in high throughput screening systems. Alkaloids will continue to have a critical role to play in the health of the Earth and of its inhabitants for the foreseeable future. They represent a significant aspect in the evolving concept of sustainable drugs and biological agents. However, only through the extensive collaboration of taxonomists, chemists, biologists, pharmacologists, formulation chemists, and clinicians can this potential be realized.

In the 12th century, according to Matthew Fox in "*Original Blessing,*" it was Saint Hildegard of Bingen who, in discussing the relationship of humankind and Nature in philosophical and practical terms, suggested that "*All nature is at the disposal of humankind. We are to work with it. For without it, we cannot survive.*" Rather like humankind, alkaloids, in all of their stunningly beautiful complexity and diversity, are an integral and essential aspect of nature with which we must work to survive.

Geoffrey A. Cordell, Ph.D.
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The Editors

John Buckingham is a former lecturer in organic chemistry at the University of London. He has been involved with the Chapman & Hall (now CRC) chemical database since its inception in 1980, initially as a Chapman & Hall employee, more recently as Editorial consultant. From the database has been produced various editions of the *Dictionary of Organic Compounds* and the *Dictionary of Natural Products* (both of which have been for some years solely electronic). In addition, he compiled (with I.W. Southon) the first edition of the *Dictionary of Alkaloids* (print only) in 1989. He is also the author of the popular science books *Chasing the Molecule* and *Bitter Nemesis; The Intimate History of Strychnine*

Keith H. Baggaley obtained his BSc (Hons) and PhD degrees from the University College of Wales, Aberystwyth followed by a post-doctoral fellowship in chemistry at the Royal Institute of Technology, Stockholm, Sweden, with Professor Holger Erdtman and Professor Torbjorn Norin. He then took up a Junior Research Fellowship with Professor David Ollis at the University of Sheffield before joining Beecham Research Laboratories in Surrey as a research chemist. At Beecham he worked on discovery projects concerned with cholesterol lowering drugs, platelet aggregation inhibitors and semisynthetic antibiotics as well as research on clavulanic acid biosynthesis. He has been an editor of the Chapman & Hall dictionaries since 1996.

Andrew D. Roberts took his BSc (Hons) degree at Trent Polytechnic, Nottingham (now Nottingham Trent University), UK 1973–1977 and completed studies in drug discovery projects at Pfizer (Sandwich) UK. He contributed to the *Dictionary of Organic Compounds* (Chapman & Hall) published in 1982 and has since been a Contributing Editor for other projects including the *Dictionary of Antibiotic Substances* (1988), *Dictionary of Drugs* (1990) and has since been an Editor on the *Dictionary of Natural Products* which was first published in 1993.

Lászloó Ferenc Szabó was born in Szentgotthárd (Hungary) on April 15, 1931 and studied in Pharmacy at University of Medicine, Budapest, 1949–54. Member of the Department of Medicinal Chemistry, later of the Department of Organic Chemistry of the Semmelweis University Budapest (scientific assistant, associate professor, ordinary professor), director of the same department 1977–1996, Ph.D. in organic chemistry, Doctor habilitatus. Research visitor at Université Libre de Bruxelles, 1972/73, several times in Merseburg (Germany). Presently professor emeritus of the Semmelweis University. Fields of activity: chemistry of natural products, mainly indole alkaloids (strychnine, strictosidine) and terpenoids (iridoids, secologanin), biogenetic formation of natural products, heterocyclic chemistry, mainly quinolizine compounds, polymer supported synthesis of small molecules, theoretical problems of organic chemistry (PMO theory, graph analysis).

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Additional data collected by contributors to the *CRC Chemical Database*

Introduction

1. COVERAGE

The *Dictionary of Alkaloids* is a comprehensive database containing over 40,000 compounds. It is a subset of the *Dictionary of Natural Products* (DNP) database. DNP is an ongoing project based on a 25-year review of the natural product literature. For the present project, the subset of DNP entries referring to alkaloids were carefully checked and reviewed and enhanced with a considerable amount of additional information relating to their natural occurrence. The intention is that the Dictionary should contain data on every known alkaloid, and various checks carried out during the compilation process indicate that it comes very close to achieving this aim. The Editors would be grateful to learn of any accidental omissions.

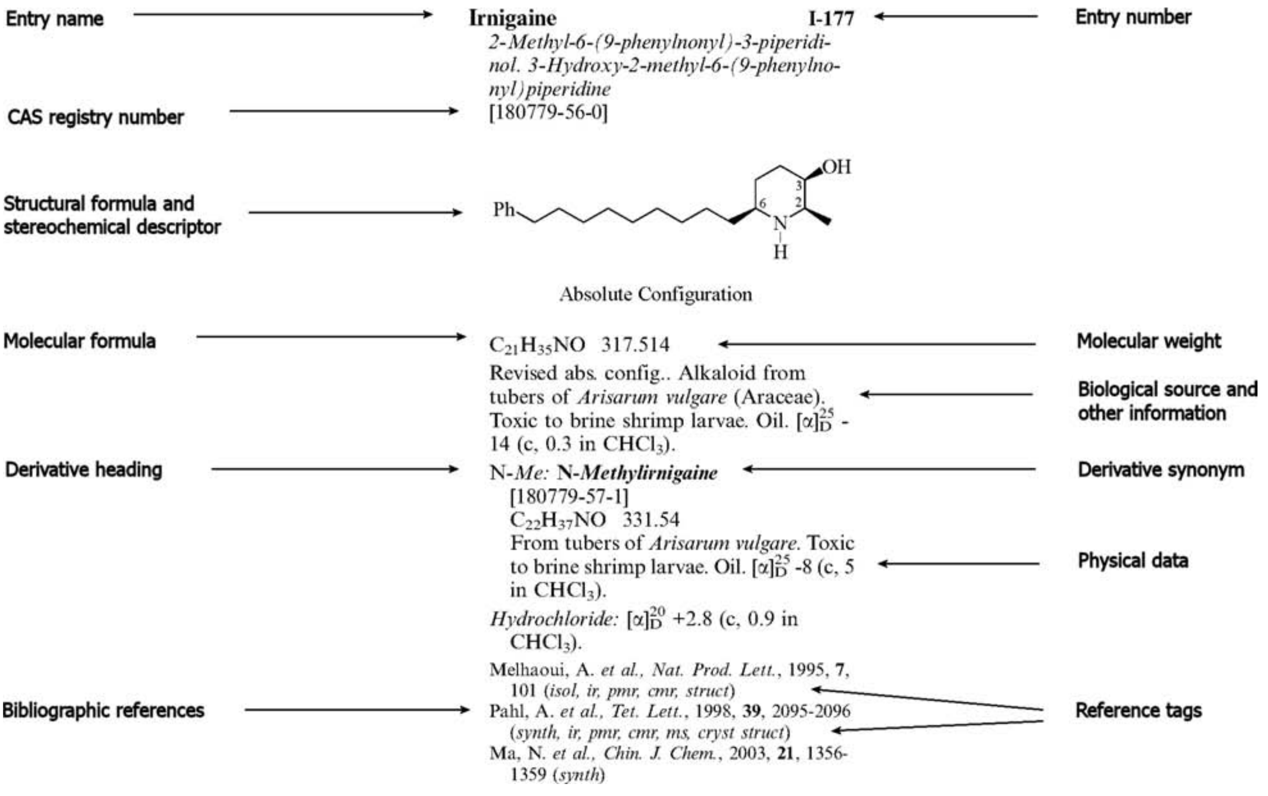
The compounds present in the Dictionary have been classified under the **Structural Types** section below. This section also includes biosynthetic information on these compound classes.

In compiling the printed version and the CD-ROM, the primary literature has been reviewed up to mid-2008.

2. ORGANISATION OF ENTRIES

The Dictionary is arranged alphabetically by entry name. Every entry is numbered to assist ready location. Many compounds are included as derivatives of main entry compounds but important derivatives have their own individual cross-referenced entries. Use of the CD-ROM indexes enables the rapid location of all compounds in the Dictionary by name or compound type, regardless of their location.

A representative dictionary entry is shown in **Figure 1.**



Irnigaine **I-177**

2-Methyl-6-(9-phenylnonyl)-3-piperidinol. 3-Hydroxy-2-methyl-6-(9-phenylnonyl)piperidine

[180779-56-0]

Absolute Configuration

$C_{21}H_{35}NO$ 317.514

Revised abs. config.. Alkaloid from tubers of *Arisarum vulgare* (Araceae). Toxic to brine shrimp larvae. Oil. $[\alpha]_D^{25}$ -14 (c, 0.3 in $CHCl_3$).

N-*Me:* **N-*Methylirnigaine***

[180779-57-1]

$C_{22}H_{37}NO$ 331.54

From tubers of *Arisarum vulgare*. Toxic to brine shrimp larvae. Oil. $[\alpha]_D^{25}$ -8 (c, 5 in $CHCl_3$).

Hydrochloride: $[\alpha]_D^{20}$ +2.8 (c, 0.9 in $CHCl_3$).

Melhaoui, A. *et al.*, *Nat. Prod. Lett.*, 1995, **7**, 101 (*isol, ir, pmr, cmr, struct*)

Pahl, A. *et al.*, *Tet. Lett.*, 1998, **39**, 2095-2096 (*synth, ir, pmr, cmr, ms, cryst struct*)

Ma, N. *et al.*, *Chin. J. Chem.*, 2003, **21**, 1356-1359 (*synth*)

FIGURE 1

2.1 CHEMICAL NAMES AND SYNONYMS

The Dictionary contains a wide range of synonyms which may be (a) those found in the primary literature, (b) *Chemical Abstracts* names, or (c) names added editorially to achieve as much consistency as possible with other closely related substances. Names corresponding to those used by CAS during the 9th and subsequent

Collective Index periods (1973-) are labelled 9CI Names. All important derivatives embedded within entries are named (but see comment on CAS nomenclature below). If a compound cannot be located immediately in the main body of the entries, it is important to use the indexes. The CD-ROM version of the Dictionary is much more highly indexed than the printed version.

The most authoritative current statement of good practice on natural product nomenclature is the document *IUPAC Recommendations 1999* (*Pure Appl. Chem.*, 1999, **71**, 587–643) the full text of which can be read on the *Dictionary of Alkaloids on CD-ROM* (access from the Windows® Start menu item or via the Help menu in the main program).

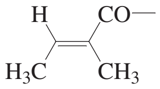
Some alkaloids have been given trivial names which duplicate those already in the literature, or which are simultaneously published for two or more non-identical substances. Where such a duplication is noticed this is indicated by the dagger symbol (‡) immediately following the name. Borderline cases, especially as between presence or absence of terminal e or suffix A or 1 are considered to constitute duplicates for this purpose.

2.1.1 Nomenclature

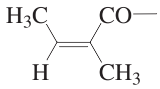
It is expected that this Dictionary will be used by a wide variety of scientists, not all of whom will be specialist organic chemists. Therefore compounds have been named so as to facilitate access to their factual data by keeping the nomenclature as simple as possible, whilst still adhering to good practice as determined by IUPAC (the International Union of Pure and Applied Chemistry). A great deal of care has been taken to achieve this aim as nearly as possible.

A much fuller description of the detailed nomenclature of individual classes of alkaloids is given in the **Structural Types** section. The following notes are of general applicability throughout the Dictionary.

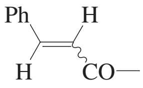
1. There are many examples in the primary literature of compounds being named in ways which are violations of good IUPAC practice, e.g. where the substituents are ordered non-alphabetically. These are not reported in their incorrect form but have been corrected.
2. The number of trivial names used for acylating substituents has been kept to a minimum but the following are used throughout the Dictionary.



Tigloyl = *E*-2-methyl-2-butenoyl



Angeloyl = *Z*-2-methyl-2-butenoyl



Cinnamoyl = 3-phenyl-2-propenoyl

3. Many other trivial appellations have from time to time appeared in the literature for other acyl groups (e.g. Senecioyl = 3-methyl-2-butenoyl, Feruloyl = 3-(4-hydroxy-3-methoxypheny1)-2-propenoyl or 4-hydroxy-3-methoxycinnamoyl).

The term **prenyl** for the common 3-methyl-2-butenyl substituent, $(H_3C)_2C{=}CHCH_2$-, is used throughout the Dictionary. Several other names for this substituent have from time to time been used and appear in the primary literature including the following:

3-Methyl-2-butenyl (systematic)
γ,γ-Dimethylallyl
3,3-Dimethylallyl
3,3-Dimethylpropenyl
Dimethallyl
Isoprenyl
Isopentenyl
β,β-Dimethylacrylyl

2.2 CAS REGISTRY NUMBERS

CAS numbers are identifying numbers allocated to each distinctly definable chemical substance indexed by CAS since 1965 (plus some retrospective allocation of numbers by CAS to compounds from earlier index periods). The numbers have no chemical significance but they provide a label for each substance independent of any system of nomenclature. They are extensively used for exchanging information between individuals and databases. The numbers take the form NNNNNN-NN-R, where the total number of digits is five or more and R is a check digit.

For practical purposes, CAS numbers have certain shortcomings arising from their free allocation, resulting in one substance having more than one potential number. Duplication may arise for one of several reasons to do with the detailed chemistry of the substance, for example tautomerism, solvent formation, partially unspecified stereochemistry. There are also replaced numbers. For this reason, Dictionary entries will often contain one or more *Additional CAS numbers* which may help the user to obtain further information about the substance, especially by online searching.

Clearly, the additional CAS numbers given in this Dictionary have to be used with care. Their inclusion in the entry is the result of an editorial decision by the Dictionary contributor that they refer to what is essentially the same substance, but this decision may be a subjective one. Care has been taken to ensure that the main CAS number given in this Dictionary for each substance is the correct one.

Further information on CAS number allocation policy can be obtained from CAS indexes or *The Organic Chemist's Desk Reference.*

2.3 STRUCTURAL FORMULAE

Every attempt has been made to present the structures of chemical substances as accurately as possible according to best current practice and recommendations of IUPAC. As much consistency as possible has been aimed at between closely-related structures, for example, all sugars are shown as Haworth formulae, and whenever possible in complex structures the rings are oriented in the standard Haworth convention so that structural comparisons can be quickly made.

2.4 MOLECULAR FORMULA AND MOLECULAR WEIGHT

The elements in the molecular formula are given according to the Hill convention (C, H, then other elements in alphabetical order). The molecular weights given are formula weights (or more strictly, molar masses in daltons) and are rounded to three places in decimals. In the case of some high molecular mass substances, such as proteins, the value quoted may be that taken from an original literature source and may be an aggregate molar mass.

2.5 PHYSICAL DATA

The Dictionary gives the following physical characteristics of substances, when available; appearance, melting point, boiling point, optical rotation, density, refractive index, solubility, p*K*a. All of these fields are searchable by numerical value (including range searching) in the CD-ROM version of the Dictionary.

2.5.1 Appearance

Organic compounds are considered to be colourless unless otherwise stated. Where the compound contains a chromophore which would be expected to lead to visible colour, but no colour is mentioned in the literature, the Dictionary entry will mention this fact if it has been noticed by the contributor. An indication of crystal form and recrystallisation solvent is often given but these are imprecise items of data; most compounds can be crystallised from several solvent systems and the crystal form often varies. In the case of the small number of compounds where crystal behaviour has been intensively studied (e.g. pharmaceuticals), it is found that polymorphism is a very common phenomenon and there is no reason to believe that it is not widespread among organic compounds generally.

2.5.2 Melting points and boiling points

The policy followed in the case of conflicting data is as follows:

a. Where the literature melting points are closely similar, only one figure (the highest or most probable) is quoted
b. Where two or more melting points are recorded and differ by several degrees (the most likely explanation being that one sample was impure) the lower figure is given in parentheses, thus Mp 139° (134–135°)

c. Where quoted figures differ widely and some other explanation such as polymorphism or incorrect identity seems the most likely explanation, both figures are quoted without parentheses, thus Mp 142°, Mp 205–206°
d. Known cases of polymorphism or double melting points are noted

Boiling point determination is less precise than that of melting points and conflicting boiling point data is not usually reported except when there appears to be a serious discrepancy between the different authors.

2.5.3 Optical rotations

These are given wherever possible, and normally refer to what the Dictionary contributor believes to be the best characterised sample of highest chemical and optical purity. Where available an indication of the optical purity (op) or enantiomeric excess (ee) of the sample measured follows the specific rotation value.*

Specific rotations are dimensionless numbers and the degree sign which was formerly universal in the literature has been discontinued.

2.6 SPECTROSCOPIC DATA

Many Dictionary entries include ultraviolet spectra which are presented in the format:

[neutral] λ_{max} 198 (log ε 1.55); 224 (sh) (log ε 0.61); 241 (sh) (log ε 0.55) (H_2O) (Berdy)

where ε is the absorption coefficient for a given UV maxima value (λ_{max}). A description of the solvent conditions used, if reported in the literature, is listed at the beginning and end of the UV data in parentheses. All peak absorptions cited are maxima unless otherwise described, e.g. shoulder/inflection (sh) and end absorption (end). In addition, UV data may be followed by the term 'Berdy' or 'DEREP' indicating from which database the data originated. The absence of these terms implies that the data was abstracted from the primary literature.

On the CD-ROM, all the λ_{max} values are indexed in the UV Maxima field and can be searched for numerically including range searching. Similarly, the solvent data associated with the UV data are indexed in the UV Solvent field.

2.7 HAZARD AND TOXICITY INFORMATION

2.7.1 General

Toxicity and hazard information is highlighted by the symbol ▶ and has been selected to assist in risk assessments for experimental, manufacturing and manipulative procedures with chemicals.

The Publishers cannot be held responsible for any inaccuracies in the reported information, neither does the omission of hazard data in the Dictionary imply an absence of this data from the literature. Widely recognised hazards are included, however, and where possible key toxicity reviews are identified in the references. Further advice on the storage, handling and disposal of chemicals is given in *The Organic Chemist's Desk Reference.*

2.7.2 RTECS® Accession Numbers

Many entries in this Dictionary contain one or more RTECS® Accession Numbers.† Possession of these numbers allows users to locate toxicity information on relevant substances from the NIOSH *Registry of Toxic Effects of Chemical Substances*, which is a compendium of toxicity data extracted from the scientific literature.

2.8 BIBLIOGRAPHIC REFERENCES

The selection of references is made with the aim of facilitating entry into the literature for the user who wishes to locate more detailed information about a particular compound. The contents of most references are indicated by reference tags (suffixes) indicating their content and in particular the stereoisomers and derivatives of the parent

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*For a recent discussion of the validity and applicability of these terms, see Gawley, R.E., *J. Org. Chem.*, 2006, **71**, 2411–2416.

† RTECS® Accession Numbers are compiled and distributed by the National Institute for Occupational Safety and Health Service of the U.S. Department of Health and Human Services of The United States of America. All rights reserved (1996).

compound which they document. The number of references cited does not indicate the relative importance of a compound; one key recent citation may supersede a number of older ones.

Journal abbreviations generally follow the practice of the Chemical Abstracts Service Source Index (CASSI), except for a short list of very well known journals where the Dictionary gives shorter abbreviations to save space (e.g. *J.A.C.S.* instead of *J. Am. Chem. Soc.*)

2.8.1 Further References

Further useful information on a variety of topics concerned with the structure, description, stereochemistry and nomenclature of organic compounds can be found in the *Organic Chemist‘s Desk Reference* (Chapman & Hall, 1995; new edition forthcoming).

3. INDEXES

There are two printed indexes:

1. A **Name Index** which lists every compound name and synonym in the Dictionary, and
2. A **Type of Compound** index listing all compounds given in the Dictionary.

The indexes refer to the entry number.

Searches on all text and numerical indexes, as well as structure and substructure searching can be carried out on the CD-ROM version of the Dictionary. For information on the Type of Compound codes used in the Type of Compound Index, please see the **Structural Types** section.

4. ABBREVIATIONS

The following is a selection of the most common Database abbreviations used:

Abbreviation	**Name**
[α]	specific rotation
abs config	absolute configuration
Ac	acetyl
acc	according
AcOH	acetic acid
Ac_2O	acetic anhydride
alk	alkaline
amorph	amorphous
amt	amount
anal	analytical applications, analysis of detection
anhyd	anhydrous
aq	aqueous
BAN	British Approved Name
bibl	bibliography
biosynth	biosynthesis
Bp	boiling point
c	concentration
ca	(*circa*) about
cd	circular dichroism
CAS	Chemical Abstracts Service
chromatog	chromatography
cmr	carbon (^{13}C) nuclear magnetic resonance
CNS	central nervous system
col	colour, coloration
coml	commercial(ly)
compd	compound
conc	concentrated
config	configuration

conformn	conformation
constit	constituent
cryst struct	X-ray crystal structure determination
d	density
dec	decomposes, decomposition
degradn	degradation
deg	degree
deriv(s)	derivative(s)
detn	detection, determination
dil	dilute, dilution
dimorph	dimorphic
diss	dissolves, dissolved
dist(n)	distil, distillation
DMF	dimethylformamide
DMSO	dimethyl sulfoxide
ee	enantiomeric excess
epr	electron paramagnetic (spin) resonance
equilib	equilibrium
esp	especially
Et	ethyl
EtOAc	ethyl acetate
EtOH	ethanol
EtOH aq	aqueous ethanol
exp	experimental
FEMA	Flavor and Extract Manufacturers' Association
fl p	flash point
fluor	fluoresces, fluorescence
formn	formation
Fp	freezing point
g	gram
glc	gas liquid chromatography
Glc	β-D-glucopyranosyl
GRAS	Generally Recognised As Safe
ham	hamster
haz	hazard
hplc	high performance liquid chromatography
hydrol	hydrolyses, hydrolysed, hydrolysis
ihl	inhalation
ims	intramuscular
INN	International Nonproprietary Name
intermed	intermediate
ipr	intraperitoneal
ir	infra-red spectrum
isol(n)	isolation, isolated
isom	isomerism, isomers, isomerises
ivn	intravenous
JAN	Japanese Accepted Name
JMAF	Japanese Ministry for Agriculture, Forestry and Fisheries
LC	lethal concentration
LD	lethal dose: LD_{50}, a dose which is lethal to 50% of the animals tested
M	molecular weight (formula weight)
manuf	manufacturer, manufactured
max	maximum
Me	methyl
MeOH	methanol

Me_2CO	acetone
MEL	maximum exposure limit
metab	metabolite, metabolism
misc	miscible
mixt	mixture
mod	moderately
Mp	melting point
ms	mass spectrum
mus	mouse
n	index of refraction, e.g. n_D^{20} for 20° and sodium light
nmr	nuclear magnetic resonance spectrum (general)
obt	obtained
oc	open cup
occup	occupational
OES	Occupational Exposure Standard
op	optical purity
ord	optical rotatory dispersion
orl	oral
Ph	phenyl (C_6H_5)
pharmacol	pharmacology
pmr	proton (^1H) nuclear magnetic resonance
polarog	polarography
polym	polymerises, polymer
ppd	precipitated
ppm	parts per million
props	properties
purifn	purification
Py	pyridine
rbt	rabbit
ref	reference
resoln	resolution
rev	review
rt	room temperature
scu	subcutaneous
sepn	separation
skn	skin
sl	slightly
sol	soluble
soln	solution
solv	solvent
sp	species (singular)
spar	sparingly
spp	species (plural)
ssp	subspecies
subl	sublimation, sublimes
synth	synthesis
tautom	tautomerism
THF	tetrahydrofuran
tlc	thin layer chromatography
TLV	Threshold Limit Value
tox	toxicity
unsatd	unsaturated
USAN	United States Adopted Name
uv	ultraviolet spectrum
v	very

var	variety
vis	visible
vol	volume

4.1 REFERENCE TAGS

The following is a selection of the most common Reference Tag abbreviations used:

Abbreviation	**Name**
abs config	absolute configuration
anal	analysis
bibl	bibliography
biosynth	biosynthesis
cd	circular dichroism
chromatog	chromatography
cmr	^{13}C nuclear magnetic resonance spectrum
config	configuration
conformn	conformation
cryst struct	X-ray crystal structure determination
deriv(s)	derivative(s)
detn	determination, detection
dta	differential thermal analysis
glc	gas-liquid chromatography
hplc	high performance liquid chromatography
ir	infrared spectrum
isol	isolation
isom	isomerism
manuf	manufacture
metab	metabolism
ms	mass spectrum
nmr	nuclear magnetic resonance spectrum
occur	occurrence
ord	optical rotatory dispersion
pharmacol	pharmacology
pmr	proton (^{1}H) nuclear magnetic resonance spectrum
props	properties (chemical or physical)
Raman	Raman spectrum
resoln	resolution
rev	review
sepn	separation
struct	structure
synth	synthesis
tautom	tautomerism
tlc	thin layer chromatography
tox	toxicity
trans	transition(s)
uv	ultraviolet spectrum
uv-vis	ultraviolet visible spectrum

5. THE DICTIONARY OF ALKALOIDS ON CD-ROM

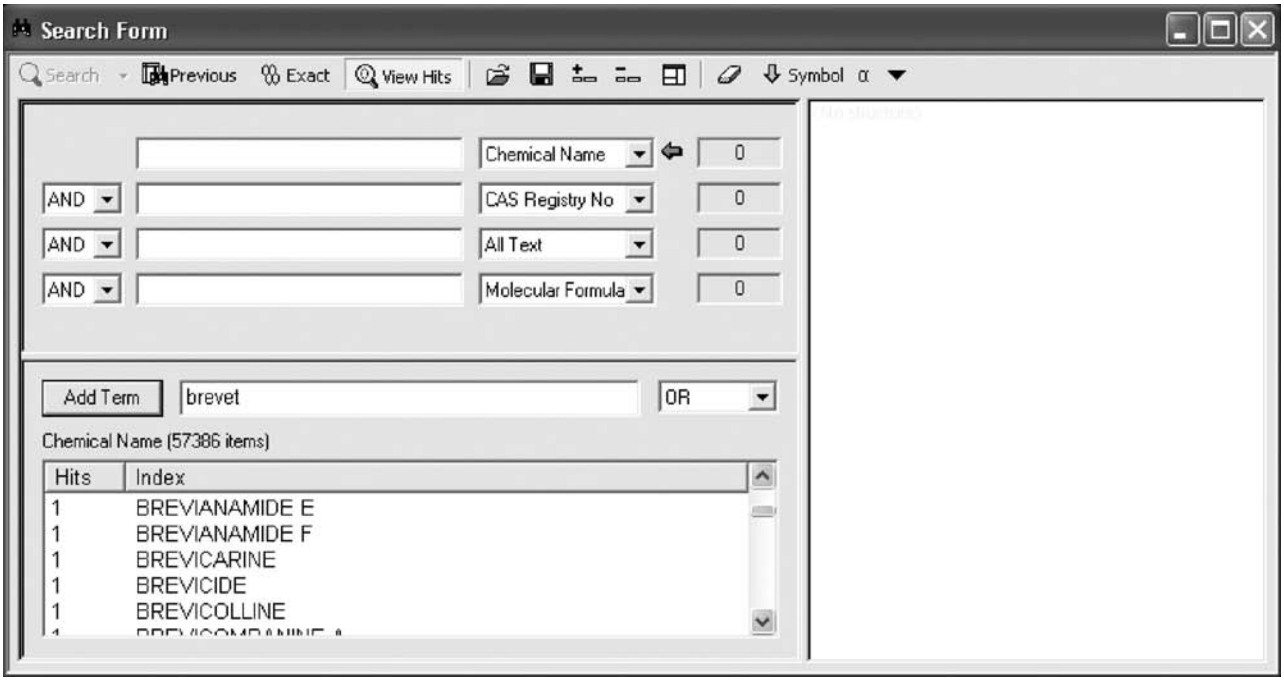
The *Dictionary of Alkaloids* is published together with a fully searchable CD-ROM. Space considerations have precluded the inclusion of indexes other than the Name Index and the Type of Compound index in the hard-copy version. By contrast, the CD-ROM contains searchable indexes on the following 35 fields:

Accurate Mass
All Entries
All Text
Biological Source
Biological Use/Importance
Boiling Point
Boiling Point Pressure
CAS Registry Number
CRC Number
Chemical Name
Density
Development Status
Dissociation Constant
Hazard & Toxicity
Hazard Flag
Ion Charge
Melting Point
Molecular Formula
Molecular Weight
Optical Rotation
Partition Coefficient (Calc.)
Percent Composition
References
Refractive Index
Rotation Conditions
RTECS Accession No.
Source/Synthesis
Supplier
Type of Compound
Type of Compound Words
Type of Organism
Type of Organism Words
Use/Importance
UV Maxima
UV Solvent

In addition to searching the above text fields, it is possible to search on structure and substructure.

Once installed, a Help file providing additional information on data content and guide to searching is available from the CRC Press folder in the Start Menu and from the Help menu on the CD-ROM.

When accessing the *Dictionary of Alkaloids on CD-ROM* the first screen that is obtained is the Search Form window (**Figure 2**).



	Chemical Name	0
AND	CAS Registry No	0
AND	All Text	0
AND	Molecular Formula	0

brevet OR

Chemical Name (57386 items)

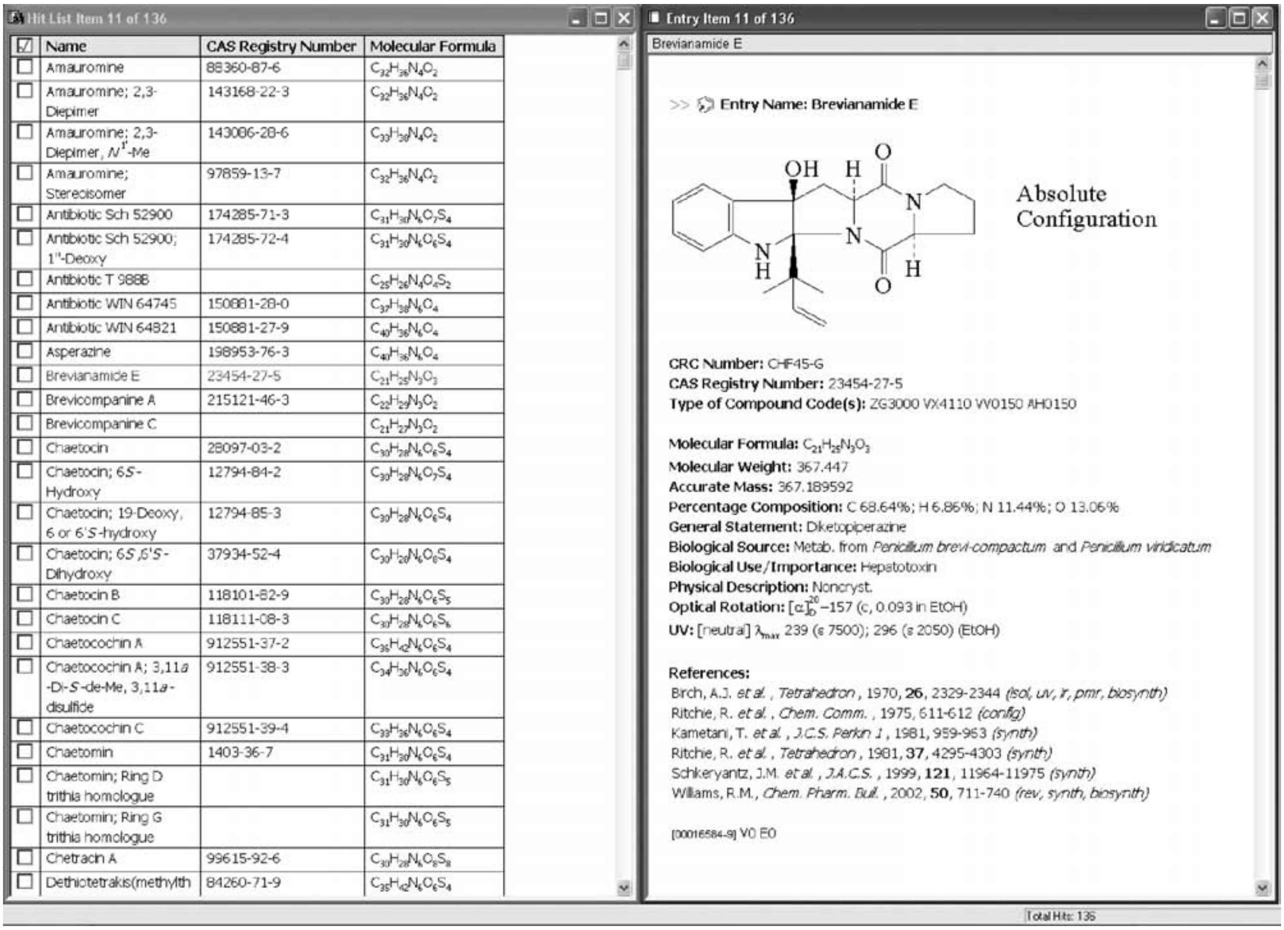
Hits	Index
1	BREVIANAMIDE E
1	BREVIANAMIDE F
1	BREVICARINE
1	BREVICIDE
1	BREVICOLLINE

FIGURE 2

The Search Form window is split in to three panes:

1. Structure Search pane - allowing structure and substructure searching
2. Search Terms pane - search from one or more of the 35 available data/text fields
3. Index pane - displays the indexed terms within a selected field

From the Search Form window design your search profile using text, structure or text/structure searching. Once your search has been performed the resultant hits are listed alphabetically by chemical name in the Hit List screen. Clicking on any one of the hits in the Hit List screen will result in that entry being displayed in the Entry Display screen (**Figure 3**).



☑	Name	CAS Registry Number	Molecular Formula
☐	Amauromine	88360-87-6	$C_{32}H_{36}N_4O_2$
☐	Amauromine; 2,3-Diepimer	143168-22-3	$C_{32}H_{36}N_4O_2$
☐	Amauromine; 2,3-Diepimer, *N*$^{1'}$-Me	143086-28-6	$C_{33}H_{38}N_4O_2$
☐	Amauromine; Stereoisomer	97859-13-7	$C_{32}H_{36}N_4O_2$
☐	Antibiotic Sch 52900	174285-71-3	$C_{31}H_{30}N_6O_7S_4$
☐	Antibiotic Sch 52900; 1''-Deoxy	174285-72-4	$C_{31}H_{30}N_6O_6S_4$
☐	Antibiotic T 988B		$C_{25}H_{26}N_4O_4S_2$
☐	Antibiotic WIN 64745	150881-28-0	$C_{37}H_{38}N_6O_4$
☐	Antibiotic WIN 64821	150881-27-9	$C_{40}H_{36}N_6O_4$
☐	Asperazine	198953-76-3	$C_{40}H_{36}N_6O_4$
☐	Brevianamide E	23454-27-5	$C_{21}H_{25}N_3O_3$
☐	Brevicompanine A	215121-46-3	$C_{22}H_{29}N_3O_2$
☐	Brevicompanine C		$C_{21}H_{27}N_3O_2$
☐	Chaetocin	28097-03-2	$C_{30}H_{28}N_6O_6S_4$
☐	Chaetocin; 6*S*-Hydroxy	12794-84-2	$C_{30}H_{28}N_6O_7S_4$
☐	Chaetocin; 19-Deoxy, 6 or 6'*S*-hydroxy	12794-85-3	$C_{30}H_{28}N_6O_6S_4$
☐	Chaetocin; 6*S*,6'*S*-Dihydroxy	37934-52-4	$C_{30}H_{20}N_6O_6S_4$
☐	Chaetocin B	118101-82-9	$C_{30}H_{28}N_6O_6S_5$
☐	Chaetocin C	118111-08-3	$C_{30}H_{28}N_6O_6S_6$
☐	Chaetocochin A	912551-37-2	$C_{36}H_{42}N_6O_6S_4$
☐	Chaetocochin A; 3,11*a*-Di-*S*-de-Me, 3,11*a*-disulfide	912551-38-3	$C_{34}H_{36}N_6O_6S_4$
☐	Chaetocochin C	912551-39-4	$C_{33}H_{36}N_6O_6S_4$
☐	Chaetomin	1403-36-7	$C_{31}H_{30}N_6O_6S_4$
☐	Chaetomin; Ring D trithia homologue		$C_{31}H_{30}N_6O_6S_5$
☐	Chaetomin; Ring G trithia homologue		$C_{31}H_{30}N_6O_6S_5$
☐	Chetracin A	99615-92-6	$C_{30}H_{28}N_6O_6S_8$
☐	Dethiotetrakis(methylth	84260-71-9	$C_{35}H_{42}N_6O_6S_4$

>> **Entry Name: Brevianamide E**

CRC Number: CHF45-G
CAS Registry Number: 23454-27-5
Type of Compound Code(s): ZG3000 VX4110 VV0150 AH0150

Molecular Formula: $C_{21}H_{25}N_3O_3$
Molecular Weight: 367.447
Accurate Mass: 367.189592
Percentage Composition: C 68.64%; H 6.86%; N 11.44%; O 13.06%
General Statement: Diketopiperazine
Biological Source: Metab. from *Penicillium brevi-compactum* and *Penicillium viridicatum*
Biological Use/Importance: Hepatotoxin
Physical Description: Noncryst.
Optical Rotation: $[\alpha]_D^{20}$ −157 (c, 0.093 in EtOH)
UV: [neutral] λ_{max} 239 (ε 7500); 296 (ε 2050) (EtOH)

References:
Birch, A.J. *et al.*, *Tetrahedron*, 1970, **26**, 2329-2344 *(isol, uv, ir, pmr, biosynth)*
Ritchie, R. *et al.*, *Chem. Comm.*, 1975, 611-612 *(config)*
Kametani, T. *et al.*, *J.C.S. Perkin 1*, 1981, 959-963 *(synth)*
Ritchie, R. *et al.*, *Tetrahedron*, 1981, **37**, 4295-4303 *(synth)*
Schkeryantz, J.M. *et al.*, *J.A.C.S.*, 1999, **121**, 11964-11975 *(synth)*
Williams, R.M., *Chem. Pharm. Bull.*, 2002, **50**, 711-740 *(rev, synth, biosynth)*

[00016584-9] V0 E0

FIGURE 3

Any comments and suggestions for inclusion may be sent to:

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Classification of Structural Types

1. DEFINITION OF AN ALKALOID

Alkaloids are a large group of nitrogen-containing secondary metabolites produced by almost every variety of organisms including humans.

The term was originally ascribed to pharmacologically active bases of plant origin, but the definition has subsequently been broadened so that it is now generally considered to include the majority of nitrogen-containing natural products with the exception of the simple amino acids and proteins, and nitrogen-containing glycosidic substances such as the aminoglycoside antibiotics. Alkaloids may be of plant, animal, insect or microbial origin. Basic properties may be weak or absent as in the various types of amide alkaloids. Not all higher plants produce alkaloids, but they are fairly widely distributed. An estimated 40% of plant families contain at least one species that is known to produce alkaloids. Traditional screening methods, e.g. using Dragendorff's reagent, may fail to detect weakly basic alkaloids.

A narrower definition has also been used, according to which the nitrogen atom(s) must be in a negative oxidation state, which excludes for example nitro and nitroso compounds. Other terms which have been used to narrow the definition include 'Imperfect alkaloids' (*Alkaloida imperfecta*), 'Pseudoalkaloid' (compounds in which the skeleton is not amino acid-derived) and 'Protoalkaloid' (bases that are amino acid-derived but acyclic, or contain rings not incorporating the amino acid-derived nitrogen). However, these terms are no longer in common use. Compounds of all of these types are in general included in the Dictionary, as well as most types of depsipeptide in which one or more amino acid residues are modified to a nitrogen heterocycle.

At the other extreme, many scientists in the life sciences/nutrition area tend to define an alkaloid as any nitrogenous toxin, including proteinaceous substances such as ptomaines. These are not included in this Dictionary.

In addition to the exclusions mentioned above, other types of nitrogenous natural product which are not covered by this Dictionary include the Sphingamines (aminolipids which are components of cerebrosides and other important biolipids) and the numerically limited but important polypyrroles, including haem, chlorophyll, etc., which can be considered as pyrrole alkaloids according to some definitions. Full entries for these are given in the parent work, *Dictionary of Natural Products.*

2. BIOSYNTHETIC CONSIDERATIONS

A great deal is now known about the biochemistry and enzymology involved in the synthesis of alkaloids by higher plants and microorganisms; because of experimental difficulties and the complexity of the ecosystems, much less is known about marine alkaloids. Purely chemical biosynthetic studies involving tracer elements are currently somewhat out of fashion, but important work in the 1970s and 1980s by several research groups delineated the framework of the biosynthetic pathways for most of the major groups of alkaloids.

In recent years, biosynthetic studies have extended into genomics, and for some important alkaloids, the whole process from nucleic acids to final assembly is now known in significant detail. The details of these pathways lie outside the scope of this Dictionary. An indication of the amount of information that is potentially available is given by the fact that, for example, eight different enzymes are involved in the construction of the relatively straightforward alkaloid Berberine, including one (berberine bridge enzyme) which is solely responsible for catalysing the insertion of the final methylene bridge into a C_{19} precursor. However, this section gives a general account of the biosynthetic and biogenetic routes to the different classes based on experimental evidence and theoretical ideas of structural interrelationships. Much more information can be obtained by consulting the biosynthesis references given in many of the individual dictionary entries.

3. NOMENCLATURE

As with all types of natural product, at least four different types of name can be distinguished. They are not given equal prominence in this Dictionary. Changes occur with time, notably associated with migrations in *Chemical Abstracts* nomenclature policy.

1. *Trivial names.* Example; Corynoxine. These convey no structural information, and if the structure of the alkaloid has not been determined, this will be the only name available. The oldest date from the first alkaloid isolations in the early nineteenth century and they are very frequently, though not always, derived from the Latin binomial or other name for the originating species, e.g. Strychnine from *Strychnos nux-vomica*. They are given prominence in this Dictionary, and every effort has been made to include every trivial name that has been used in the past. The names have the advantage that since they convey no structural information, they are unchanged if there is a structure revision of the alkaloid, a common event.

   There are a number of duplications of trivial names in the literature, and these are indicated by the sign ‡.

   Trivial names for at least plant-based alkaloids have traditionally ended in *–ine*.
2. *Systematic names.* Example: Methyl 6′-ethyl 1,2,2′,3,6′,7′,8′,8′*a*-octahydro-α-(methoxymethylene)-2-oxospiro[3*H*-indole-3,1′(5′*H*-indolizine]-7′-acetate, (α*E*,1′*S*,6′*S*,7′*S*,8′a*S*)- is the current CAS name for Corynoxine. The names are unambiguous and put natural products on the same footing as other organic compounds, but are of course cumbersome and typically not interpretable in terms of a recognizable structure. They are also subject to change if CAS nomenclature policy changes. These names are given in the Dictionary for relatively small molecules, and the name used to head the entry may be a systematic one if it is short and convenient. For larger molecules, such as Corynoxine, where this Dictionary does not give the systematic (CAS) name, it can be readily accessed using the CAS registry numbers that are given throughout the Dictionary. Systematic names, where they are shown in an entry, are usually presented without their stereodescriptors. These can be seen by examining the structure diagram or by consulting CAS.

   There are many cases in which CAS numbering does not correspond with the biogenetic schemes used by most natural products scientists, and which are given prominence in this Dictionary. Workers in the field are aware of such discrepancies which are inevitable. Another common complication is that structural changes which to the alkaloid specialist are minor (e.g. introduction of a methylenedioxy group) cause profound changes to the CAS name, in this case because the methylenedioxy being is recognised as an additional heterocyclic ring fusion. For further details, see the compound type descriptions given below and the individual dictionary entries.
3. *Semisystematic names.* Examples are the skeletons represented by Corynoxan and Ergoline. IUPAC gives lists of these and directions for introducing new ones. These semisystematic parents can be modified by operators such as nor-, abeo-, and seco-, etc. CAS still uses this type of name for some types of alkaloid such as ergolines (e.g. Ergometrinine = 9,10-Didehydro-*N*-(2-hydroxy-1-methylethyl)-6-methylergoline-8-carboxamide), but has abandoned it for many other alkaloid classes, e.g. Corynoxans, in favour of systematic nomenclature. In general, the construction of semisystematic names of this type has not found universal support in view of the discovery of ever more structurally complex types of natural product, and also of the potential complexities caused by different authors deriving new parent skeletons in different ways. These names are not in general given in this Dictionary.
4. *'Semitrivial' names.* These are names which are derived by appending a systematically-derived operator to a trivial parent. Examples are 8-(1,1-Dimethylallyl)confusameline and *N*-Cyano-*sec*-pseudostrychnine. Such names are widespread, but are best avoided because of the possibilities for confusion, especially when there is a structure revision, or where there is more than one numbering scheme in use for the parent skeleton. Trivial names should be preferred. These semitrivial names are however, reported throughout the Dictionary where they are found in the literature. Where a semitrivial name is no longer accurate because there has been a structure revision, a note is given in the dictionary entry, and reference is often given to the possibility of confusion caused by the use of different numbering schemes.

4. PRINCIPAL LITERATURE SOURCES

4.1 REVIEW SERIES

Progress in the Chemistry of Organic Natural Products, formerly *Fortschritte der Chemie Organischer Naturstoffe*, (various editors), Springer Verlag, 1938- (***'Prog. Chem. Org. Nat. Prod.'***).

The leading annual review series for all types of natural product, although recent volumes contain fewer contributions on alkaloids.

Alkaloids, Chemistry and Biology (ed. Manske, R.H.F., then Rodrigo, R., then Brossi, A. then Cordell, G.A.), Academic Press, then Wiley, then Elsevier, 1949- (**'*Alkaloids*'**).

The leading review series devoted to alkaloids. Referred to in CAS as *'Alkaloids, N.Y.'*, or *'Alkaloids (Academic Press)'*, (but no longer abstracted)

Alkaloids, Chemical and Biological Perspectives (ed. Pelletier, S.W.), Pergamon/Elsevier, 1983–2000 ('***Alkaloids Chem. Biol. Perspect***.').
Another good review series, although no longer published.

Natural Product Reports, Royal Society of Chemistry, 1984-.
Timely, succinct and authoritative reviews; coverage depends on the availability of authors for particular topics.

Boit, H.-G., *Ergebnisse der Alkaloid-Chemie bis 1960*, Akademie Verlag, 1961.
Comprehensive compilation of all alkaloid isolations to 1960.

4.2 RECENT BOOKS

Raffauf, R.F., *Plant Alkaloids: A Guide to their Discovery and Distribution*, Food Products Press, 1996
Alkaloids: Biochemistry, Ecology and Medical Applications (eds. Roberts, M.A. *et al.*), Plenum Press, 1998
Compr. Nat. Prod. Chem. (ed. Kelly, J.W.), Elsevier, 1999, **4**
Hesse, M., *Alkaloids: Nature's Curse or Blessing?,* Wiley-VCH, 2002
Aniszewski, T., *Alkaloids – Secrets of Life*, Elsevier, 2007
Modern Alkaloids: Structure, Isolation, Synthesis and Biology (eds. Fattorusso, E. *et al.*), Wiley-VCH, 2007

5. TYPE OF COMPOUND CLASSIFICATION SCHEME

All alkaloids in the Dictionary carry one or more Type of Compound codes in the format VX1234, where VX is an invariable code denoting alkaloids (other codes starting with V refer to other types of natural product that can be found in the *Dictionary of Natural Products*. Some alkaloids carry additional non-alkaloid codes).

These codes are shown against the headings below and can be searched in the CD-ROM version of the Dictionary or in the parent *Dictionary of Natural Products* (DVD or web version). The VX code numbers assigned to an alkaloid type have no intrinsic significance. They are allocated so as to make the groups and subgroups appear in a reasonable biochemical sequence, and to provide gaps in the numerical order so that newly discovered types of alkaloid can be inserted.

Use of these codes in searching is complementary to searching by substructure. In some classes of alkaloid (such as the various types of steroidal alkaloid), the structures are fairly homogeneous, but in other classes (for example, the *Daphniphyllum* alkaloids), a wide variety of carbon skeleton may be produced by variation of an underlying biogenetic scheme. In such cases, substructure searching cannot locate all of the possibilities and the Type of Compound coding is of great value. Some alkaloids carry more than one code where they are of an intermediate type, or contain structural fragments that can be assigned to two different categories.

Biogenetically and structurally the alkaloids are diverse, and it is usual to discuss them in terms of biogenetic origin rather than purely on the basis of structural features. The classical plant alkaloids were from an early date recognised at being mostly derived from amino acids, notably ornithine (→ pyrrolidines, tropanes, etc.), lysine (→ piperidines), phenylalanine, and tryptophan (→ many alkaloids including the numerous and structurally diverse indole alkaloids). The order of Type of Compound codes in the first edition of this Dictionary followed this general scheme, which was also followed in most treatises on alkaloids. However, the subsequent discovery of many more diverse types of alkaloid, especially those of microbial and marine origin, has blurred these traditional biogenetic categories. New categories have now been inserted where it seemed appropriate on structural grounds, but these may not necessarily be biogenetically related to the established alkaloid types. To take one example, the Ericamycins (VX3900) have been placed at the end of the isoquinoline alkaloids because they contain a condensed isoquinoline nucleus, but they are of polyketide origin and have little in common biogenetically with the 'traditional' isoquinoline alkaloids. Even some well-established plant alkaloids were found on investigation to be polyketide in origin. The best-known example is Coniine, a long-known piperidine alkaloid which, however, is not lysine-derived. Other examples include Pinidine and (probably) Carpaine.

Much less is known about the biogenesis of marine alkaloids than their terrestrial counterparts because of experimental difficulties and the complexity of the ecosystems. Where structural similarities exist between certain marine alkaloids and their terrestrial counterparts, this is frequently indicated in the following sections, but this should not be taken to imply that their biosynthesis takes place by identical routes. There may be cases of biochemical parallelism arising from convergent evolution. In most instances the relevant information is simply not yet available for the marine alkaloids.

Details are now being uncovered about formerly unsuspected enzyme systems, which superimpose new biosynthetic possibilities on top of the traditional routes, thus blurring the traditional alkaloid subtypes.

Foremost among these are the 'Diels-Alderases' (not confined to alkaloids) which are capable of catalysing the formation of new carbon skeletons from known types. The Type of Compound categories in the database are therefore subject to future revision in the light of new research results.

Brief descriptions of the alkaloid types follow. These are not meant to be definitive, as the amount of information available for most groups of alkaloid is too great to summarise in such a brief introduction. However, the Dictionary as a whole will point the user to the key literature sources for every group; either via the general reviews given below under each category, or by going to the individual dictionary entries for the alkaloids in each group and from there to the references cited in the entry.

Herbert, R.B., *Nat. Prod. Rep.*, 2003, **20**, 494–508 (*rev*, *biosynth*)
Oikawa, H. *et al.*, *Nat. Prod. Rep.*, 2004, **21**, 321–352 (*rev*, *Diels-Alder enzymes*)
Moore, B.S., *Nat. Prod. Rep.*, 2005, **22**, 580–593; 2006, **23**, 615–629 (*rev*, *biosynth*)

Simple acyclic amine alkaloids with one n (VX0100)

These include simple amines of mostly widespread biological occurrence such as **Choline** and **Ethylamine**. Various miscellaneous polyamines are categorised under VX9000, miscellaneous acyclic alkaloids.

Simple guanidines (VX0150)

This heading covers low molecular weight guanidinoid bases, many of marine origin. Their high polarity demands special isolation techniques. The guanidine or modified guanidine group is common as a structural component of higher molecular weight alkaloids, including hybrid polyketide alkaloids and peptide-alkaloids which are classified elsewhere below.

Berlinck, R.G.S., *Prog. Chem. Org. Nat. Prod.*, 1995, **66**, 119–26 (*rev*)
Nagasawa, K. *et al.*, *Chem. Rec.*, 2003, **3**, 201–211 (*rev*, *synth*)
Berlinck, R.G.S. *et al.*, *Nat. Prod. Rep.*, 2005, **22**, 516–520; 2008, **25**, 919–954 (*revs*)

Nitriles, isonitriles and related compounds (VX0200)

Compounds containing the -NC, -NCS and -NHCHO groups frequently occur together and are biogenetically related. Compounds having the same carbon skeleton are usually included in the same entry. It now appears that the thiocyanates are central in their biosynthesis.

Edenborough, M.S. *et al.*, *Nat. Prod. Rep.*, 1988, **5**, 229–246 (*rev*, *isonitriles*)
Fleming, F.F., *Nat. Prod. Rep.*, 1999, **16**, 597–606 (*rev*, *nitriles*)
Garson, M.J. *et al.*, *Nat. Prod. Rep.*, 2004, **21**, 164–179 (*rev*)

Simple isobutylamide alkaloids (VX0220); other simple amide alkaloids (VX0250)

Simple isobutylamide amides are common plant constituents, VX0250 includes a variety of other simple amides such as the marine **Variceramides** and a wide range of other miscellaneous amides. The most intensively studied are the capsaicinoids, such as **Capsaicin**, which are responsible for the pungent flavours of capsicum peppers (Solanaceae) and related plants.

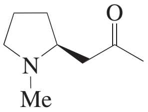
Suzuki, T. *et al., Alkaloids*, 1984, **23**, 228–300 (*rev, capsicum alkaloids*)
Cordell, G.A. et al., *Ann. Pharmacother.*, 1993, **27**, 330–336 (*rev*)

Azo and azoxy alkaloids (VX0280)

These are not very numerous and their classification as alkaloids is borderline. They include toxic (carcinogenic) metabolites such as **Cycasin**.

Simple pyrrolidine alkaloids (VX0300, VX0380)

Several simple pyrrolidine alkaloids are known from plants. These include **Hygrine** and **Stachydrine**. In *Nicandra physaloides*, Hygrine is biosynthesised from ornithine. Condensation of two ornithine units with acetoacetate gives **Cuscohygrine**. Other alkaloids containing a pyrrolidine ring include **Ficine** (in which the pyrrolidine ring is attached to a flavone nucleus), and **Brevicolline** (in which it is attached to a β-carboline unit). Clearly the biogenesis of these molecules requires other precursors.



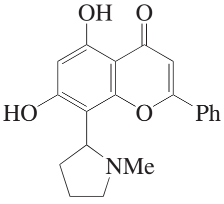
Hygrine

Other simple pyrrolidine alkaloids may arise by different biosynthetic pathways. The kainoids, e.g**. α-Kainic acid**; **Domoic acid,** are a group of non-proteinogenic pyrrolidinedicarboxylic acids. α-Kainic acid was first isolated from a rhodophyte alga but has since been found in terrestrial organisms. The kainoids are biosynthesised from glutamate and geranyl pyrophosphate, while many others are presumably proline-derived. Simple pyrrolidines based on a longer-chain skeleton such as the **Broussonetines** are biosynthesised analogously to sphingosines. Many other compounds indexed under miscellaneous pyrrolidine alkaloids (VX0380) contain a pyrrolidine function as part of a larger structure.

Massiot, G. *et al., Alkaloids,* 1986, **27**, 270–332 (*rev*)
Parsons, A.F., *Tetrahedron*, 1996, **52**, 4149–4174 (*kainoids*, *rev*)

CHROMONE AND FLAVONOID ALKALOIDS (VX0340, VX0350)

A structure consisting of a pyrrolidine, piperidine or pyridine ring linked to the A ring of chromone is referred to as a chromone alkaloid. This group of compounds can be sub-divided into two types, namely those in which the chromone nucleus exists as Noreugenin (5,7-Dihydroxy-2-methylchromone) — indexed as chromone alkaloids VX0340 — and those which bear a phenyl substituent at *C*-2 (indexed as flavonoid alkaloids, VX0350). The former group is typified by **Rohitukine** and **Schumannificine**. Typical flavonoid alkaloids include **Ficine** and **Vochysine**. Compared with the noreugenin-related alkaloids, which have only been isolated from the plant families Meliaceae and Rubiaceae, the flavonoid alkaloids are more widely distributed throughout the higher plants.

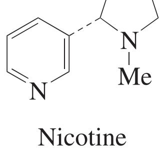


Ficine

Houghton, P.J. *et al., Alkaloids,* 1987, **31**, 67–100 (*chromone alkaloids*; *rev*)

NICOTINE-LIKE ALKALOIDS (VX0360)

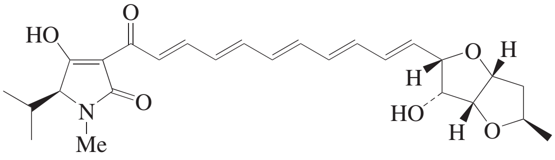
This is a small group of well-known pharmacological and toxicological importance, **Nicotine** being the major alkaloid of tobacco. The pyridine ring in nicotine is derived from nicotinic acid and the pyrrolidine ring from *N*-methylpyrrolinium derived from arginine or ornithine via putrescine. The genomics and enzymology of nicotine biosynthesis are well studied. **Nornicotine** is a deleterious tobacco constituent which is a major cause of carcinogenesis through *N*-nitrosation.



Nicotine

TETRAMIC ACIDS (VX0390)

These are longer-chain pyrrolidines exemplified by the halogenated **Aurantosides** and **Rubrosides** from sponges (microbial products). A range of nonhalogenated tetramic acids has been isolated from terrestrial microorganisms, such as **Erythroskyrin** and the **Lipomycins**. They are polyketide in origin.

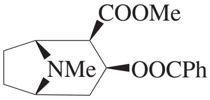


Erythroskyrin

Schobert, R. *et al., Bioorg. Med. Chem.*, 2008, **16**, 4203–4221 (*rev*)

TROPANE ALKALOIDS (VX0400)

These are characteristic constituents of the Solanaceae. Almost all of them are esters of mono-, di-, and trihydroxytropanes, with a wide variety of hydroxylation patterns (see for example **Calystegines**). In view of their pharmacological importance (**Cocaine**, **Atropine** and relatives) their synthesis and biosynthesis has been much studied since the nineteenth century. They are derived from ornithine and acetoacetate. One or two condensed structures occur, e.g. **Bellendine**, **Darlingine**.



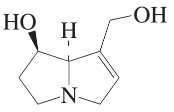
Cocaine

Hemschiedt, T., *Top. Curr. Chem.*, 2001, **209**, 175–206 (*rev*, *biosynth*)
Gossauer, A., *Prog. Chem. Org. Nat. Prod.*, 2003, **86**, 1–188 (*rev*)
Biastoff, S., *et al., Alkaloids,* 2007, **64**, 49–102 (*Calystegines*)

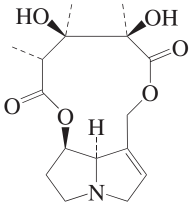
PYRROLIZIDINE ALKALOIDS (VX0440, VX0500, VX0520)

These occur in species of the *Senecio* genus, and elsewhere in the Asteraceae and Fabaceae. They have been shown to be responsible for the toxic effects, particularly liver damage, in livestock grazing on pastures infested by these species, and are of public health interest in human liver disease. In view of this they have been extensively reviewed. Many, and perhaps the majority, of pyrrolizidine alkaloids occur in the plant as *N*-oxides, the *N*-oxide function being lost during isolation. Toxicity appears to be the result of oxidation *in vivo* to pyrrole derivatives. Pyrrolizidine alkaloids enter the food chain and become antifeedants in animal species such as butterflies.

The majority of pyrrolizidine alkaloids are either relatively simple esters formed from a pyrrolizidine base, the necine, exemplified by **Retronecine**, and a necic acid, such as senecioic (VX0440), or more complex cyclic esters formed between a necine and a necic acid (VX0500), an example being **Monocrotaline**. The necic acids are probably derived from an amino acid (e.g. isoleucine), rather than acetate or mevalonate. **Callosine** represents an unusual variation.



Retronecine



Monocrotaline

The category of miscellaneous pyrrolizine alkaloids includes some unusual pyrrolizidines from totally different sources, e.g. **Antibiotic PF 1018** from a fungus, **Nitropolyzonamine** from a millipede, and the cyclic polysulfide **Cassipourine** from a higher plant.

Robins, D.J., *Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 115–204 (*rev*)
Wróbel, J.T., *Alkaloids*, 1985, **26**, 327–384 (*rev*)
Powell, R.G. *al*, *Alkaloids Chem.Biol. Perspect.,* 1990, **8**, 320–338 (*rev*, *Loline group*)
Naturally Occurring Pyrrolizidine Alkaloids, (ed. Rizk, A.-M.), CRC Press, 1991
Hartmann, Y. *et al., Alkaloids Chem. Biol. Perspect.,* 1994, **9**, 155–233 (*rev*)
Robins, D.J., *Alkaloids*, 1995, **46**, 1–61 (*rev*, *biosynth*)

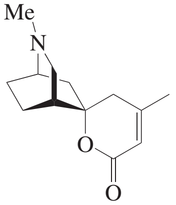
Hartmann, T. *et al., Top. Curr. Chem.*, 2001, 209, 207–244 (*biosynth and metabolism in plants and insects*)
Liddell, J.R., *Nat. Prod. Rep.*, 2002, **19**, 773–781 (*rev*)
Jiang, Y. *et al.*, *Asian J. Pharmacodyn. Pharmacokinet.*, 2006, **6**, 187–192 (*tox*)

SIMPLE PIPERIDINE ALKALOIDS; MISCELLANEOUS PIPERIDINE ALKALOIDS (VX0680, VX0700)

Like the pyrrolidines, these alkaloids may arise by different biosynthetic routes, so the class is structural rather than biosynthetic. Some may be derived from lysine, acetate, acetoacetate, etc., in analogous fashion to the simple pyrrolidine alkaloids. The majority of the alkaloids in this group are plant-derived. **Piperidine** itself is a lysine-derived alkaloid.

All these structural types have their analogues among the pyrrolidine alkaloids, and while it is tempting to assume biosynthesis from lysine it may not in all cases be true; **Coniine**, for example, is acetate-derived. The longer-chain **Batzellasides**, present in sponges, are iminoglycosides structurally related to the intensively-studied terrestrial iminosugars such as **Nojirimycin**, evidently with the incorporation of a fatty-acid derived fragment.

Dioscorine, from *Dioscorea hispida*, provides a fascinating example of the unexpected in alkaloid biosynthesis. At first sight it seems plausible to postulate that it may be formed from lysine and a polyketide fragment. However, lysine is not a precursor, and it would appear that Dioscorine is formed from nicotinic acid and, probably, a polyacetate unit.

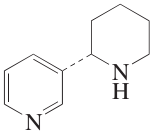


Dioscorine

Strunz, G.M. *et al., Alkaloids*, 1985, **26**, 89–184 (*rev*)
Fodor, G.B. *et al.*, *Alkaloids Chem. Biol. Perspect.,* 1985, **3**, 1–90 (*rev*)
Schneider, M.J., *Alkaloids Chem.Biol. Perspect.*,1993, **10**, 155–300 (*rev*)
Andersen, R.J. *et al.*, *Alkaloids Chem. Biol. Perspect.,* 1996, **10**, 301 (*rev*, *3-alkylpiperidines*)

ANABASINE ALKALOIDS (VX0620)

These are piperidine homologues of the nicotine group (VX0360 above). They also occur in *Nicotiana* spp., in *Anabasis* spp. and others. The biosynthesis is, at least in its major features, analogous to that of the nicotine group, with lysine → cadaverine → *N*-methyl-Δ^1-piperideine replacing ornithine → putrescine → *N*-methyl-Δ^1-pyrrolideine. **Anabasine** has been isolated from marine animals and insects, as well as plants.



Anabasine

However, the piperidine ring in **Anatabine**, from *Nicotiana glutinosa*, appears not to be derived from lysine or from a polyacetate precursor; instead, both rings are derived from nicotinic acid.

LOBELIA-TYPE ALKALOIDS (VX0660)

These have no analogy among the pyrrolidine alkaloids. An example is **Lobelanine**.

Felpin, F.X. *et al., Tetrahedron*, 2004, **60,** 10127–10153 (*rev*)

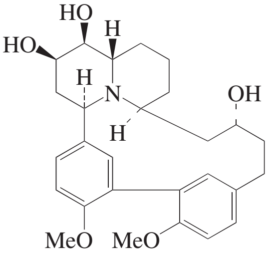
XESTOSPONGINS (VX0690)

These are a group of exclusively marine-elaborated piperidines. Their biosynthesis would appear to imply the involvement of a C_{10} dialdehyde equivalent as hypothesised for the Manzamine group (VX2250) below, and they appear closely related to intermediates postulated in the Baldwin scheme.

Baldwin, J.E. *et al.*, *Tet. Lett.*, 1992, **33**, 2059–2062 (*biosynth*)

LYTHRACEAE ALKALOIDS (VX0760)

These are characterised by several unusual structural features. **Lythrancine** contains a quinolizidine ring system attached to a diphenyl residue, one of the benzene rings in which is derived from cinnamic acid. Other alkaloids in this group contain a diphenyl ether grouping, e.g. **Decaline**, and others a piperidine ring instead of a quinolizidine ring, e.g. **Lythranidine**. These alkaloids have not been studied recently, and their biosynthesis has not been fully worked out. It involves lysine as source of the quinolizidine or piperidine ring, and phenylalanine as precursor of one of the aromatic rings.



Lythrancine

The numbering system adopted here for the lactonic Lythraceae alkaloids (e.g. Decaline) is the one generally accepted, and corresponds closely to that for piperidine and quinolizidine metacyclophane alkaloids (e.g. Lythranidine, Lythrancine). The carbon atoms that correspond in biogenetic origin to the three alkaloid types thus maintain corresponding numbers. CAS originally employed stereoparent names for these alkaloids, but now uses systematic nomenclature; in each case the numbering is different.

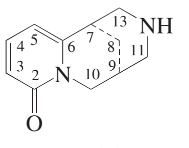
Golebiewski, W.M. *et al., Alkaloids*, 1981, **18**, 263–273 (*rev*)
Fuji, K., *Alkaloids*, 1989, **35**, 155–176 (*rev*)

QUINOLIZIDINE ALKALOIDS (VX0900, VX0920, VX0940, VX0960, VX0980)

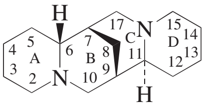
Quinolizidine alkaloids are sometimes reviewed alongside pyrrolizidine and indolizidine alkaloids under the joint heading ‘Izidines’. The well-known alkaloids which have been long known were isolated from higher plants, particularly the Fabaceae, but the quinolizidine nucleus also occurs in some marine alkaloids and amphibian toxins.

Two-ring quinolizidine alkaloids (VX0900) come from various sources and range from simple bases such as **Epiquinamide**, from a frog toxin, to more elaborated examples such as the marine **Pictamine** and the Fabaceae alkaloid **Epilupinine**, to others which are clearly seco-derivatives of larger alkaloids, e.g. **Cadiamine**. A few relatively simple marine quinolizidine alkaloids are known such as **Pictamine** and the **Clavepictines**. The **Saraines** are more complex sponge products classified under miscellaneous quinolizidines (VX0980), together with **Halichlorine**, a popular synthetic target, and the **Petrosines**, further examples of dimeric alkaloids in which the units are linked in a medium-sized aliphatic ring.

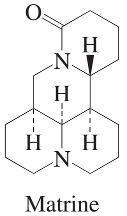
Of the three-ring alkaloids (VX0920) the most characteristic is **Cytisine**; other alkaloids such as **Angustifoline** having a carbon substituent are clearly intermediate between Cytisine and the four-ring alkaloids. The **Tsukushinamines** (which actually have four rings) represent an unusual variation.



(-)-Cytisine



(-)-Sparteine



Matrine

The four-ring alkaloids (VX0940) are the most studied group. Fusion of an additional ring onto the cytisine skeleton produces the **Sparteine** type with potentially increased (C_2) symmetry. Both enantiomers of Sparteine and many of its relatives occur naturally, the enantiomers (and sometimes the racemate) often being characterised in the older literature under different names. The symmetry properties mean that the nomenclature and numbering of Sparteine derivatives is confusing, especially since in the past many alkaloids have sometimes been poorly named. Every effort has been made to regularise the nomenclature and numbering, and to show the absolute configurations correctly.

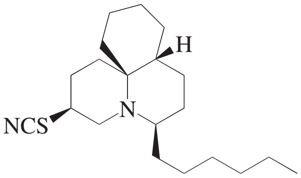
Another type of four-ring alkaloid is represented by **Matrine** and its stereoisomers (**Isomatrine**, **Allomatrine**, **Sophoridine**, **Darvasamine**). These groups contain some dimers, e.g. **Dithermamine**.

The miscellaneous group (VX0980) includes some alkaloids with larger structures, for example **Jamine** and **Panamine** (each six rings).

Howard, A.S., *Alkaloids*, 1986, **28**, 183–308 (*rev*)
Aslanov, Kh.A., *Alkaloids*, 1987, **31**, 118–193 (*rev*)
Robins, D.J. *et al., Alkaloids*, 1995, **46**, 1–61 (*rev, synth*)
Ohmiya, S. *et al.*, *Alkaloids*, 1995, **47**, 2–115 (*rev*, *lupine alkaloids*)
Michael, J.P., *Alkaloids*, 2001, **55**, 91–258 (*rev*)
Michael, J.P., *Nat. Prod. Rep.*, 2008, **25**, 139–165 (*rev*)

CYLINDRICINE ALKALOIDS (VX0960)

The Cylindricine/Fasicularine/Lepadiformine alkaloids (VX0960) are a small cluster of marine alkaloids containing the perhydrobenzo[*i*]quinolizine nucleus and ring-contracted homologues, plus some terrestrial alkaloids which are loosely related structurally.



Fasicularine

Biosynthetic studies do not yet appear to have been carried out. Benzologous structures have been proposed for a small group of terrestrial alkaloids (Menispermaceae) related to **Cohirsine**.

Weinreb, S.M., *Chem. Rev.*, 2006, **106**, 2531–2549 (*rev*, *synth*)

AZEPINE ALKALOIDS (VX1000)

These are mostly microbial (or marine, presumably microbial) products; the exceptions are fungal pigments such as **Chalciporone** and its congeners. Marine alkaloids include the **Bengamides**, which are thought to be symbiotic products deriving from bacterial fatty acids, cyclised lysine and a 4-carbon diketide.

NICOTINIC ACID DERIVED ALKALOIDS (VX1020); OTHER PYRIDINE ALKALOIDS (VX1040)

The number of small alkaloids derived by the transformation of nicotinic acid is limited. There are, however, a large number of terpenoid ester alkaloids in which nicotinic acid itself esterifies a variety of terpenoid alcohols, for example dihydro-β-agarofurans (e.g. the **Cangorins** and many others).

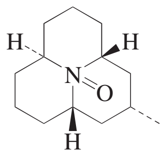
Arecoline, from betel nuts, and **Ricinine**, from the castor oil plant, are clearly derivable from nicotinic acid; in the case of Ricinine this has been established.

Strunz, G.M. *et al., Alkaloids*, 1985, **26**, 89–184 (*rev*)
Fodor, G. *et al., Alkaloids Chem. Biol. Perspect.,* 1985, **3**, 1–90 (*rev*)
Schneider, M.J., *Alkaloids Chem. Biol. Perspect.,* 1993, **10**, 155–300 (*rev*)
Almeida, A.M.P. *et al.*, *Quim. Nova*, 1997, **20**, 170–185 (*rev*, *alkylpyridines from sponges*)
Sepčić, K., *J. Toxicol., Toxin Rev.*, 2000, **19**, 139–160 (*rev*, *alkylpyridinium compounds from sponges*)
Liao, L.M., *Alkaloids*, 2003, **60**, 287–343 (*rev*, *sesquiterpene pyridine alkaloids*)

9*B*-AZAPHENALENE ALKALOIDS (VX1120)

(Systematically pyrido[2,1,6-*de*]quinolizines). This small piperidine-based group is exemplified by **Coccinelline**, the defensive agent of the common ladybird, *Coccinella septempunctata*, and **Porantherine**, from the shrub

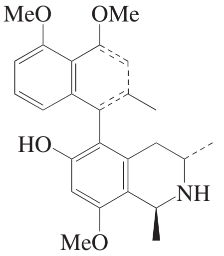
Poranthera corymbosa. The insect alkaloids appear to be genuine insect metabolites which are biosynthesised from a lipid chain forming the outer perimeter, plus glutamine as the preferred nitrogen source.



Coccinelline

Naphthalene-isoquinoline alkaloids (VX1140)

This group is isolated mainly from the plant family Ancistrocladaceae, with some isolations from the Dioncophyllaceae. Several skeletal types are known and are based on the point of linkage between the two ring systems, e.g. 5,1′-coupled alkaloids (**Ancistrocladine**, **Dioncophylline C**), 5,8′-coupled (**Korupensamine A**), 7,1′-coupled (**Ancistrocladisine**, **Dioncophylline A**), 7,3′-coupled (**Ancistrocladidine**), 7,6′-coupled (**Dioncophylline B**), etc. These alkaloids are chiral due to diastereoisomerism at the methyl groups and in the biaryl linkage due to restricted rotation. They are biosynthesised via construction of a naphthalenoid portion onto monomeric dihydroisoquinolines.

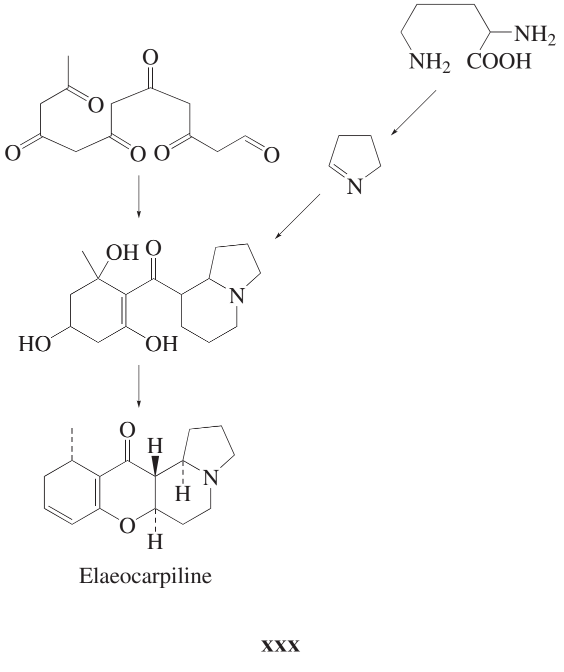


Ancistrocladine

Bringmann, G. *et al., Alkaloids*, 1986, **29**, 141–184; 1995, **46**, 128–272 (*revs*)
Bringmann, G. *et al.*, *Tetrahedron*, 2007, **63**, 1755–1761 (*biosynth*)

Elaeocarpus alkaloids (VX1160)

These are a series of mostly indolizidine-based alkaloids from Far-eastern *Elaeocarpus* spp. A proposed biosynthetic scheme which was suggested in 1969, and which apparently lacks experimental evidence, is through the condensation of a twelve-carbon polyketide chain with a 1-pyrroline derived from ornithine. Alternatively, the whole skeleton may be polyacetate derived.

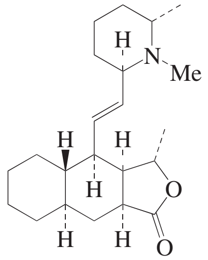


Elaeocarpiline

Johns, S.R. *et al.*, *Aust. J. Chem.*, 1969, **22**, 793–800 (*biosynth*)
Johns, S.R. *et al., Alkaloids*, 1973, **14**, 325–346 (*rev*)

GALBULIMIMA ALKALOIDS (VX1240)

These are a numerically limited class of alkaloids e.g. **Himbacine,** based on the elaboration of a piperidine theme, and which are found in *Galbulimima* (*Himantandra*) spp. (Himantandraceae). A biosynthetic scheme for these alkaloids was suggested in 1967 which proposed their construction from a common polyacetate precursor. Synthetic studies have been carried out to provide a biomimetic route along these lines, however, direct experimental proof is still lacking.

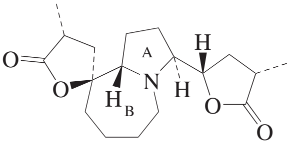


Himbacine

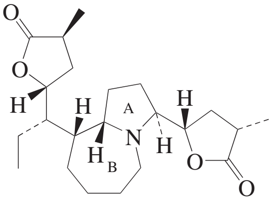
Shah, U. *et al., Total Synthesis of Galbulimima Alkaloids*, VDM Verlag Dr. Muller, Aktiengesellschaft, 2008 (*rev, synth*)

STEMONA ALKALOIDS (VX1260)

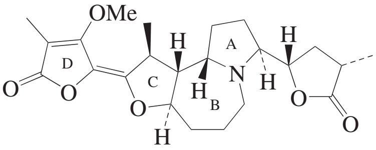
These represent a unique type of alkaloid isolated only from the family Stemonaceae (monocots). Three main types are recognised, the **Croomine**, **Stichoneurine** and **Protostemonine** types, although a further subdivision into 11 subtypes can be made. Biosynthetic studies of Stemona alkaloids have not been reported, but a scheme based on a terpenoid origin of the C and D rings and a spermidine origin of the A ring has been proposed by Seger, and an alternative scheme involving a polyketide-geranate condensation by Pyne and co-workers.



Croomine



Stichoneurine A

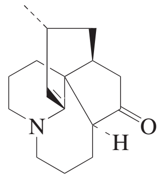


Protostemonine

Pilli, R.A. *et al.*, *Nat. Prod. Rep.*, 2000, **17**, 117–128 (*rev*)
Seger, C. *et al.*, *Chem. Biodiversity*, 2004, **1**, 265–279 (*biosynth*)
Pilli, R.A. *et al., Alkaloids,* 2005, **62**, 77–173 (*rev*)
Greger, H., *Planta Med.*, 2006, **72**, 99–113 (*rev*)
Pyne, S.G. *et al.*, *Maejo Int. J. Sci. Technol.*, 2007, **1**, 157–165 (*rev, biosynth*)

LYCOPODIUM ALKALOIDS (VX1280)

These are constituents of the club mosses (Lycopodiaceae). Whereas the earliest proposal concerning their biosynthesis implicated two C_8 units derived from acetate, it was later established that two lysine units are involved. Numerous skeletal variants are known, all of which can be related to the Lycopodine skeleton; older examples are **Fawcettidine** and **Serratinine**. More recently some intriguing new skeletons such as those in the **Lyconadines**, **Lyconesidine A**, the **Lycopladines** and **Neohuperzinine** have been found.

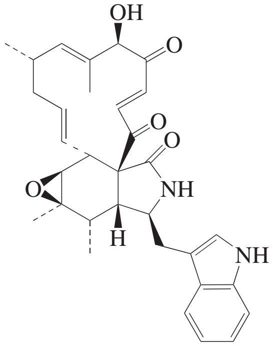


Fawcettidine

Maclean, D.B., *Alkaloids*, 1985, **26**, 241–298 (*rev*)
Blumenkopf, T.A. *et al., Alkaloids Chem. Biol. Perspect.,* 1985, **3**, 185–240 (*rev*)
Ayer, W.A., *Nat. Prod. Rep.*, 1991, **8**, 455–464 (*rev*)
Ayer, W.A., *Alkaloids*, 1994, **45**, 233–274 (*rev*)
Ma, X. *et al.*, *Nat. Prod. Rep.*, 2004, **21**, 752–772 (*rev*)
Peng, J. *et al., Alkaloids*, 2005, **61**, 1–57 (*rev*)

CYTOCHALASAN ALKALOIDS (VX1300)

Cytochalasins are metabolites of several different and unrelated fungi, including some marine actinomycetes. They are characterised structurally by the presence of a perhydroisoindolone system fused to a macrocyclic ring of 11, 13 or 14 atoms. The macrocycle may be a carbocycle, a lactone or a carbonate. In addition, the isoindole ring carries either a phenyl or an indolyl substituent at position 10; the latter group includes the **Chaetoglobosins**. Cytochalasins possess a range of distinctive biological properties; these include inhibition of cytoplasmic cleavage leading to polynucleate cells, nuclear extrusion and the inhibition of cell mobility. Biosynthetically, cytochalasins arise from phenylalanine or tryptophan and a polyketide derived from acetate and methionine. They have not been reviewed recently.

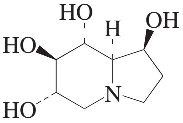


Chaetoglobosin A

Pendse, G.S., *Recent Advances in Cytochalasans*, Chapman & Hall, 1987

INDOLIZIDINE ALKALOIDS (VX1360)

These are a significant class of plant alkaloids, e.g. **Castanospermine**, an important biologically active enzyme inhibitor and a major synthetic target, and **Swainsonine**, biosynthesised from lysine.



Castanospermine

A large number of indolizidine alkaloids known are amphibian skin toxins, of which the greatest number are 5,8-disubstituted, e.g. **Indolizidine 203A**. These are now all known to be of dietary origin, possibly entering the frogs through arachnid and insect prey. Many of these are available only in traces and have currently been characterised only by mass spectroscopic methods, with a number of structures uncertain or incomplete. They are homologous with the ring-expanded quinolizidine series (see VX0900 above), and other related skeletons by ring enlargement. There are no conclusive studies on the biosynthesis of these related series of amphibian and related toxins, but a polyketide origin is plausible.

A few simple indolizidines (e.g. the **Stellettamides**) have been isolated from sponges.

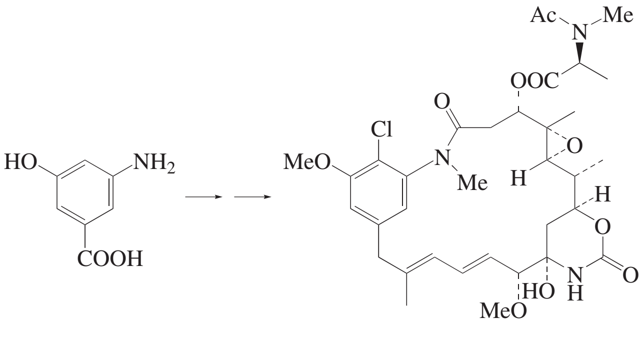
Howard, A.S., *Alkaloids*, 1986, **28**, 183–308 (*rev*)
Elbein, A.E. *et al., Alkaloids Chem. Biol. Perspect.,* 1987, **5**, 1–54 (*rev*)
Takahata, H. *et al., Alkaloids*, 1993, **44**, 189–256 (*rev*)
Michael, J.P., *Nat. Prod. Rep.*, 2004, **21**, 625–649; 2005, **22**, 603–626; 2008, **25**, 139–165 (*revs*)
Daly, J.W. *et al., J. Nat. Prod.*, 2005, **68**, 1556–1575 (*amphibian toxins*)
Amat, M. *et al.*, *Angew. Chem. Internat. Ed. Engl.*, 2008, 47, 3348–3351 (*amphibian toxins*)

Simple anthranilic acid alkaloids (VX1460)

A number of diverse structural groups of alkaloid are derived biogenetically from anthranilic acid, the major ones being the quinolone, acridine and quinazoline groups categorised under their respective headings. The number of unelaborated anthranilic acid alkaloids is small and includes **Damascenine** from *Nigella damascena*. Biosynthetically, the alkaloid is derived from anthranilic acid (chorismate derived), which is then hydroxylated and methylated.

Maytansinoids (VX1470)

The maytansinoids are a group of ansa macrocyclic lactams originally isolated from three plant families (Euphorbiaceae, Celastraceae, Rhamnaceae), and subsequently isolated from a soil bacterium *Actinosynnema pretiosum*, other microorganisms and mosses. They are homologous with the **Ansamitocins** from microorganisms, and may be derived from plant-associated fungi. They show strong antitumour activity and are biosynthesised from the simple aromatic precursor 3-amino-5-hydroxybenoic acid, arising from the chorismate pathway, which is substituted by a polyketide chain and then amide ring formation.



Maytansine

Cassady, J.M. et al., *Chem. Pharm. Bull.*, 2004, **52**, 1–26 (*rev*)

Simple quinolines (VX1480); Furanoquinolines (VX1520); Pyranoquinolines (VX1540); Miscellaneous quinoline alkaloids (VX1580)

The majority of simple quinoline alkaloids are from higher plants, but a variety of simple heteroaromatic quinolines (VX1480) have been isolated from various marine sources, including **2-Heptyl-4-hydroxyquinoline** from a marine pseudomonad, and **4,8-Quinolinediol** from cephalopod ink. Plant alkaloids include **Echinopsine** and the phenethyl-quinoline, **Cusparine**. The plant-derived furanoquinoline (VX1520) (e.g. **Platydesmine**), and pyranoquinoline (VX1540) alkaloids (e.g. **Flindersine**) are straightforwardly derived from simple alkylquinolines (especially prenyl-substituted) by cyclisation. There are also more elaborated hydrogenated quinolines, especially the **Lepadins** from tunicates and flatworms.

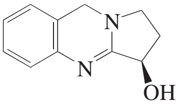
Bryozoans contain a number of simple quinoline-quinone pigments and there are also the **Trididemnic acids** from ascidians. Simple hydrogenated quinolines also occur in amphibian toxin mixtures, for example the numerous ***Dendrobates* Alkaloids**. This extensive series of alkaloids occurs in amphibian skin extracts and in tunicates, flatworms and insects (myrmicine ants), in a mixture which includes hydrogenated quinolines, and structural variants such as indolizidines (VX1360, see for further information).

Macrorine, from *Macrorungia longistrobus*, is obviously derived from anthranilic acid and histidine.

Grundon, M.F., *Alkaloids Chem. Biol. Perspect.,* 1988, **6**, 339–522 (*rev*)
Fernandes da Silva, M.F. *et al., Alkaloids*, 2007, **64**, 139–214 (*rev*)
Michael, J.P., *Nat. Prod. Rep.*, 2008, **25**, 166–189 (*rev*)

QUINAZOLINE ALKALOIDS (VX1600)

These include **Vasicine**, first isolated in 1888 from *Adhatoda vasica*, and **Rutaecarpine**, from *Euodia rutaecarpa*; this latter base is clearly derived from tryptophan and anthranilic acid. Quinazoline alkaloids have been isolated from several plant families as well as from microorganisms, fungi and animal spp. **Febrifugine** is a pharmacologically important (antimalarial) member of the group. A number of simple quinazolines also occur, as well as **Bouchardatine**, which is a quinazoline-indole dimer. They have been well reviewed; see also Tryptoquivalines (VX6030) below.

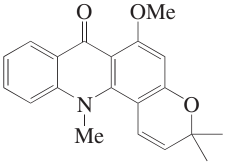


Vasicine

Johne, S., *Prog. Chem. Org. Nat. Prod.*, 1984, **46**, 159–218 (*rev*)
Johne, S., *Alkaloids*, 1986, **29**, 99–140 (*rev*)
Mhaske, S.B., *Tetrahedron*, 2006, **62**, 9787–9826 (*rev*)
Michael, J. *et al.*, *Nat. Prod. Rep.*, 2008, **25**, 166–187 (*rev*)

ACRIDONE ALKALOIDS (VX1620-VX1690)

These are higher plant alkaloids characteristic of the Rutaceae, and are biosynthesised from anthranilic acid by elaboration of an additional malonate-derived aromatic ring. The simple acridones (VX1620) may be exemplified by **Xanthevodine** and by a large number of alkaloids in which the nucleus is prenylated followed frequently by formation of a furano- or pyranoacridine ring system, e.g. **Acronycine**. Biosynthesis of the nucleus is from anthranilic acid and a malonate fragment. The **Acrimarines** are acridone-coumarin dimers (VX1690).

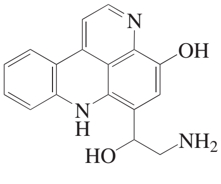


Acronycine

Gerzon, K. *et al., Alkaloids*, 1983, **21**, 1–28 (*rev*)
Grundon, M.F., *Alkaloids Chem.Biol. Perspect.*, 1988, **6**, 339–522 (*rev*)
Tillequin, F. *et al., Alkaloids Chem. Biol. Perspect.,* 1998, **12**, 1–102 (*Acronycines*, *rev*)
Skaltsounis, A. *et al., Alkaloids*, 2000, **54**, 259–377 (*rev*)
Michael, J.P., *Nat. Prod. Rep.*, 2008, **25**, 166–187 (*rev*)

PYRIDO[2,3,4-*KL*]ACRIDINES (VX1700)

This is a group of exclusively marine alkaloids which includes the **Kuanoniamines**, the **Ascididemins**, the **Cystodytins**, the **Styelsamines**, the **Varamines** and others. The isolation of some of them from a variety of organisms argues for a microbial origin, but it could alternatively be a case of convergent evolution. They are biosynthesised from common amino acids.

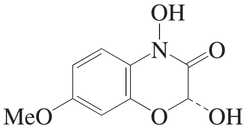


Styelsamine A

Molinski, T.F., *Chem. Rev.*, 1993, **93**, 1825–1838 (*rev*)
Ding, Q. *et al.*, *Curr. Med. Chem.*, 1999, **6**, 1–27 (*rev*)
Salomon, C.E. *et al.*, *Mar. Biol. (Berlin)*, 2001, **139**, 313–319 (*biosynth*)
Moore, B.S., *Nat. Prod. Rep.*, 2006, **23**, 615–629 (*rev*)

1,4-Benzoxazin-3-one alkaloids (VX1720)

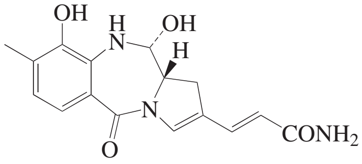
2,4-Dihydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one (known as DIMBOA) is the main representative of this group of alkaloids which have plant hormone significance. DIMBOA itself protects the maize plant against corn borer attack. They usually occur in the plant as glucosides, but cell injury releases a glucosidase which catalyses hydrolysis to the 2-hydroxy derivatives. All four oxygen atoms in DIMBOA arise by incorporation of molecular O_2.



DIMBOA

Benzodiazepine alkaloids (VX1760)

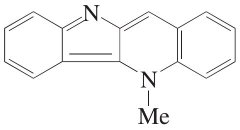
This is a growing class of microbial metabolites typified by **Anthramycin** and others. One or two, e.g. **Aplysepine**, are of marine origin; apparently no plant alkaloids with this skeleton are known to date. They are biosynthesised from amino acids via kynurenine and its derivatives.



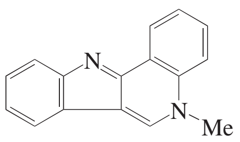
Anthramycin

Cryptolepine alkaloids (VX1800)

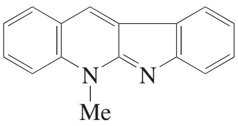
Cryptolepine (5-Methyl-5*H*-quindoline) is the most prominent representative of this small group isolated from *Cryptolepis* spp. The parent alkaloid, 10*H*-Indolo[3,2-*b*]quinoline (**Quindoline**), has been isolated from *Cryptolepis sanguinolenta*. Two isomeric skeletons (**Isocryptolepine**, **Neocryptolepine**) were also obtained. A further variant represented by **Cryptoheptine** is doubtful. The marine **Communesins** (currently classified under miscellaneous alkaloids VX9400) contain the Neocryptolepine skeleton embedded in a polycyclic ring system. No biosynthetic studies of these skeletons have been carried out, but a derivation from indole and anthranilic acid can be envisaged.



Cryptolepine



Isocryptolepine

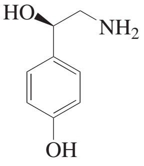


Neocryptolepine

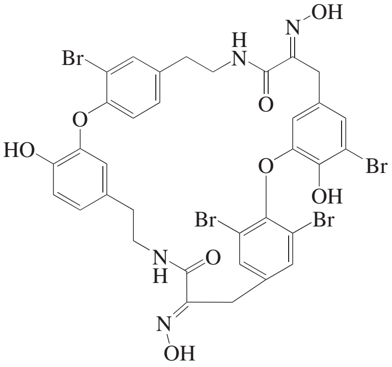
SIMPLE PHENETHYLAMINE ALKALOIDS (VX2000, VX2005, VX2008, VX2015)

Alkaloids derived from phenylalanine or tyrosine represent an extremely large and varied major subdivision of the alkaloids, ranging from simple β-phenylethylamine derivatives to the much more complex structures exemplified by the alkaloids of the Amaryllidaceae and the very numerous isoquinoline alkaloids.

The simplest derivatives of phenylalanine or tyrosine are the β-phenylethylamines, which are presumably obtained by decarboxylation and obvious oxidative/alkylation stages, and which are widespread among plant alkaloids (e.g. **Mescaline**) and elsewhere. Compounds showing side-chain oxygenation (VX2005) include alkaloids from higher plants, such as **Macromerine**, as well as animal hormones such as **Adrenaline** and **Octopamine**, which is an endometabolic neurotransmitter of molluscs. Brominated compounds (VX2008) such as the **Purpuramines** and the **Bastadins** are common in marine organisms. These are biosynthesised from the simple brominated tyrosines.



Octopamine



Bastadin 9

Lundström, J., *Alkaloids*, 1989, **35**, 77–154 (*rev*)
Peng, J. *et al., Alkaloids*, 2005, **61**, 59–262 (*rev, marine bromotyrosine alkaloids*)
Bentley, K.W., *Nat. Prod. Rep.*, 2006, **23**, 444–463 (*rev*)

EPHEDRA ALKALOIDS (VX2010)

This is a small, and important, group of low molecular weight alkaloids centred on **Ephedrine** and its relatives, isolated from *Ephedra* spp. (Ma Huang) and showing strong physiological activity. They carry a side-chain amino or substituted amino substituent. This structural feature is common in higher molecular weight alkaloids.

Ma Huang and the Ephedra Alkaloids, (ed. Karch, S.B.), Springer/Humana Press, 2007 (*book*)

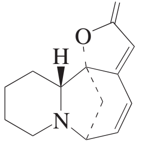
CINNAMIC ACID AMIDES (VX2020)

***cis*-** and ***trans*-Fagaramide**, **Herclavine** and **Subaphylline** are simple members of this series, which are mostly isolated from terrestrial plants. These amides are typically derived from a *trans*-cinnamic acid; **Astrophylline** is an example of an *N*-*cis*-cinnamoyl derivative. Simple cinnamate residues are scarcer among marine alkaloids. Examples are found in the **Tunichromes**, for which phenylalanine can function as a biosynthetic precursor.

Taylor, S.W. *et al.*, *Chem. Rev.*, 1997, **97**, 333–346 (*rev*, *tunichromes*)

SECURINEGA ALKALOIDS (VX2100)

This small group of polycyclic alkaloids occurs in the Euphorbiaceae. The biosynthesis of these alkaloids, which is not readily apparent, has been shown to involve tyrosine and lysine in the case of **Securinine**. Alkaloids of both enantiomeric series occur naturally, sometimes in closely related plants.

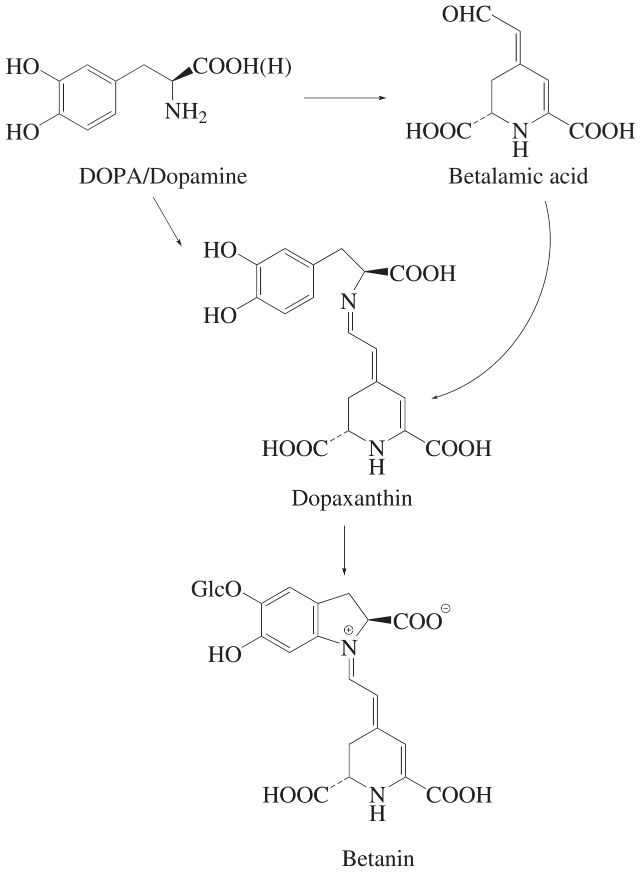


Securinine

Snieckus, V., *Alkaloids*, 1973, **14**, 425–506 (*rev*)

Betalain alkaloids (VX2140)

This is a group of zwitterionic water-soluble alkaloidal pigments whose distribution is limited to the order Caryophyllales of the dicots, (more or less coterminous with the older term Centrospermae), for which they have been used as a taxonomic marker, plus some basidiomycete fungi. **Betanin** (the red pigment of beetroot) is the best-known example, other examples include various flower pigments instead of anthocyanins. Both halves of the molecule are biosynthesised from DOPA/Dopamine via Dopaxanthin; the formation of the upper unit, Betalamic acid, involves an enzymatic aromatic ring fission process.



Stintzing, F. *et al.*, *Trends Food Sci. Technol.*, 2007, **18**, 514–525 (*rev*)

ISOQUINOLINE ALKALOIDS (VX2200-VX2400)

This is an extremely large group of mainly higher plant alkaloids, although one or two groups of isoquinolinoid marine alkaloids, notably the Manzamine group (VX2250) are also interpolated into the listing.

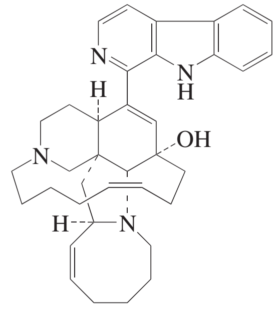
Shamma, M., *The Isoquinoline Alkaloids*, Academic Press, New York, 1972
Shamma, M. *et al.*, *Isoquinoline Alkaloid Research, 1972–1978*, Plenum Press, New York, 1978
Krane, B.D., *J. Nat. Prod.*, 1982, **45**, 377–384 (*rev*)
Lundström, J., *Alkaloids*, 1983, **21**, 255–328 (*rev*)
Phillipson, J.D. *et al.*, *The Chemistry and Biology of Isoquinoline Alkaloids*, (eds. Phillipson, J.D. *et al.*), Springer, 1985
Menachery, M.D., *J. Nat. Prod.*, 1986, **49**, 745–778 (*rev*)
Baker, B.J. *et al., Alkaloids Chem. Biol. Perspect.,* 1996, **10**, 357–407 (*rev*, *marine isoquinolines*)
Bentley, K.W., *Nat. Prod. Rep.*, 2006, **23**, 444–463 (*rev*, *revs cited therein*)

Simple isoquinoline alkaloids (VX2200)

This group includes simple isoquinolines with (e.g. **Salsoline**) or without (e.g. **Anhalamine**) a *C*-1 substituent, and various quinones (**Mimosamycin**, **Renierone)**. Marine examples are restricted to some bases related to **Renierol** and the **Cribrostatins**.

MANZAMINE ALKALOIDS (VX2250)

This fairly extensive group (a typical representative is **Manzamine A**) is exclusively of marine origin and represents the most structurally complex and characteristic type of marine alkaloid for which a biosynthetic scheme has been proposed. Their biosynthesis has been postulated to involve the condensation of tryptamine with one or more C_3 units and one or more straight-chain C_{10} dialdehyde equivalents, followed by an enzyme-assisted Diels-Alder cyclisation. The origin of the C_{10} and C_3 units is uncertain, but it has been suggested that they could arise by oxidative fission of a hydroxylated fatty acid. The full biosynthetic scheme is shown in the reviews below and more elaborately in the companion *Dictionary of Marine Natural Products.*



Manzamine A

Baldwin, J.E. *et al.*, *Tet. Lett.*, 1992, **33**, 2059–2062 (*biosynth*)
Tsuda, M. *et al.*, *Heterocycles*, 1997, **46**, 765–794 (*rev*)
Baldwin, J.E. *et al.*, *Chem. Eur. J.*, 1999, **5**, 3154–3161 (*biosynth*)
Hu, J.F. *et al., Alkaloids*, 2003, **60**, 207–285 (*rev*)
Thomas, R., *Nat. Prod. Rep.*, 2004, **21**, 224–248 (*rev*, *biosynth*)

BENZYLISOQUINOLINE ALKALOIDS (VX2320)

The simple benzylisoquinoline skeleton is derived from two molecules of tyrosine, via DOPA, and is the precursor of a wide variety of alkaloids in categories listed below, belonging to numerous different ring systems. The alkaloids with the unmodified benzylisoquinoline skeleton consist mainly of 1,2,3,4-tetrahydrobenzylisoquinolines, e.g. **Reticuline**, of central importance in the elaboration of other alkaloids, and their fully aromatic analogues, e.g. **Papaverine**. Alkaloids with a carbon substituent at *C*-2′, such as **Canadaline**, may be regarded as ring-opened berberines. There are also some benzylisoquinolines in which a pyrrolidine ring is attached to *C*-4, e.g. **Macrostomine**. The isolation of one or two marine benzylisoquinoline alkaloids (**Imbricatine**; **Theoneberine**) is noteworthy.

Deulofeu, V. *et al., Alkaloids*, 1968, **10**, 401–461 (*rev*)

PSEUDOBENZYLISOQUINOLINE ALKALOIDS (VX2330)

The term pseudobenzylisoquinoline alkaloid is used to describe a benzylisoquinoline skeleton in which the pendant aromatic ring is oxygenated at *C*-2′, *C*-3′ and *C*-4′. These alkaloids are derived biogenetically from protoberberinium salts by *C*8-*C*8*a* bond scission. **Polycarpine**, **Taxilamine** and **Ledecorine** are typical examples.

BISBENZYLISOQUINOLINE ALKALOIDS (VX2340–VX2400)

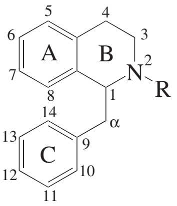
This large group of alkaloids is composed of two benzylisoquinoline units attached to each other by one, two, or three bonds. In most cases the units are joined via ether linkages, but carbon-carbon bonds between the benzyl groups are also known. The monomeric units involved are mainly hydroxylated or methoxylated benzylisoquinolines, although aporphine units occur in many alkaloids, and a few contain a proaporphine component. The alkaloids may be subdivided into the five following major groups (the classification, proposed by Shamma, contains at least 28 subgroups). All alkaloids classified here are composed of unmodified benzylisoquinoline units. Dimeric alkaloids containing aporphine, proaporphine, or otherwise modified benzylisoquinoline components are discussed under separate headings).

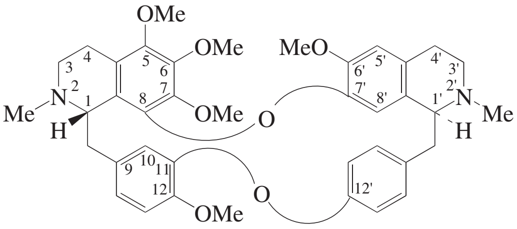
CAS used to employ a number of stereoparent skeletons, such as Berbaman, Thalicberan, Tubocuraran, in naming the cyclic bisbenzylisoquinoline alkaloids, but these have now been replaced by systematic nomenclature. Trivial nomenclature is given prominence in this Dictionary, but the main semisystematic parent skeletons are shown below. Care is needed in numbering the two benzylisoquinoline residues. In a few cases, CAS has in the past applied the primes to the opposite residue to that proposed in the Shamma-Moniot convention. The latter is used in this Dictionary.

The Shamma-Moniot convention is as follows;

1. The numbering system for a bisbenzylisoquinoline half of the dimer is as shown below. The lower aromatic ring, namely ring C, is always numbered so as to assign the smallest numbers to the substituents on that ring
2. Each bisbenzylisoquinoline half of the dimer is described in terms of its oxygenation pattern. The more highly oxygenated bisbenzylisoquinoline half constitutes the left hand side of the dimer. The right hand side of the dimer is given prime numbering.

For an example see the structure of Hernandezine below.





Hernandezine with Shamma-Moniot convention numbering

Shamma, M. *et al., Heterocycles*, 1976, **4**, 1817–1824 (*Shamma-Moniot numbering convention*)
Buck, K.T., *et al., Alkaloids*, 1987, **30**, 1–222 (*rev*)
Schiff, P.L., *J. Nat. Prod.*, 1997, **60**, 934–953 (*rev, revs cited therein*)

Bisbenzylisoquinoline alkaloids containing aryl links only (VX2340)

The bark of *Popowia pisocarpa* has yielded a group of alkaloids which contain a single aromatic linkage between *C*-11 and *C*-11′. See the entry for **Pisopowetine**. **Isopythaldine** and **Isopyruthaldine** represent another type in which the two benzylisoquinoline groups are joined by methylene bridges.

Bisbenzylisoquinoline alkaloids containing one ether link (VX2360)

The ether linkage is in most cases between *C*-11 and *C*-12′, as in **Dauricine**. However, other attachments are known, e.g. between *C*-10 and *C*-11′, as in **Vanuatine**, between *C*-10 and *C*-7′, as in **Malekulatine** and **Ambrimine**, and between *C*-11 and *C*-7′, as in **Neferine**.

Bisbenzylisoquinoline alkaloids containing one aromatic link and one or two ether links (VX2370, VX2390)

These alkaloids are mainly based on the **Rodiasine** and **Tiliacorine** skeletons.

Bisbenzylisoquinoline alkaloids containing two ether links (VX2380)

These are the most numerous. The largest subgroup containing two ether linkages possesses the berbaman skeleton, exemplified by **Berbamine**, which contains ether linkages between *C*-8 and *C*-7′, and between *C*-11 and *C*-12′. Almost as large as the berbaman group is the oxyacanthan group, e.g. **Oxyacanthine**, which contains ether linkages between *C*-7 and *C*-8′, and between *C*-11 and *C*-12′. Smaller groups include the **Thalicberine** (*C*-8 to *C*-6′

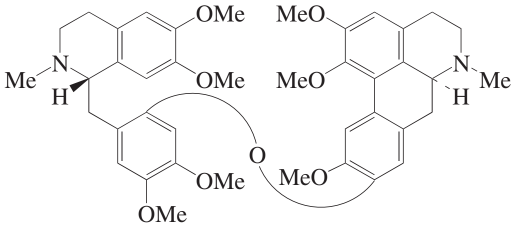
and *C*-11 to *C*-12′), **Thalidasine** (*C*-8 to *C*-5′ and *C*-11 to *C*-12′), and **Thalmine** (*C*-7 to *C*-5′ and *C*-11 to *C*-12′) types. All of these types contain ether linkages between the benzyl rings and between the aromatic rings of the tetrahydroisoquinoline component. The **Tubocurarine** sub-group contains ether linkages between the benzyl ring of one unit and the aromatic ring of the isoquinoline component of the other. Other linkages between benzyl and isoquinoline rings are also known.

BISBENZYLISOQUINOLINE ALKALOIDS WITH THREE ETHER LINKS (VX2400)

These include alkaloids with 6′,7-epoxyoxyacanthan (e.g. **Trilobine**), 7,8′-epoxyoxyacanthan, and 8,12′-epoxytubocuraran skeletons.

BENZYLISOQUINOLINE-APORPHINE DIMERS (VX2700)

Some alkaloids consist of a benzylisoquinoline unit attached to an aporphine unit, through a single ether linkage. Of these, **Thalicarpine** is typical.



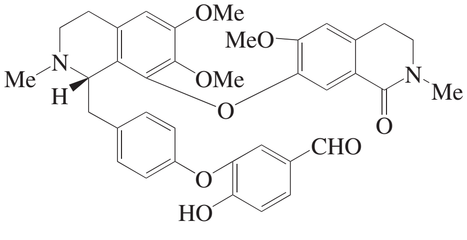
Thalicarpine

Miscellaneous bisbenzylisoquinoline-related alkaloids (listed under their component monomeric units) include those containing a dienone ring in one of the isoquinoline moieties (e.g. **Repanduline**), some with an aporphine unit attached to a pavine component (e.g. **Pennsylpavine)**, those with degraded benzylisoquinoline units (e.g. **Baluchistanamine**) or with a proaporphine unit (e.g. **Epiberbivaldine**), and **Cancentrine**, which is really a combination of cularine and morphinan components.

Buck, K.T. *et al., Alkaloids*, 1987, **30**, 1–222 (*rev*)
Schiff, P.L., *Alkaloids Chem.Biol. Perspect.,*1987, **5**, 271–638; 2000, **14**, 1–234 (*revs*)

SECOBISBENZYLISOQUINOLINE ALKALOIDS (VX2430)

The secobisbenzylisoquinolines are degraded alkaloids in which one of the benzylisoquinoline units is cleaved between the *C*-1 and the α-carbon atom. A typical example is **Baluchistanamine**, the apparent biogenetic precursor of which is Oxyacanthine. Different oxidation states are found; aldehyde lactams (e.g. **Baluchistanamine**, **Punjabine**), lactam esters (e.g. **Punjabine**, **Curacautine**) or aldehyde amines (**Jhelumine**, **Chenabine**).

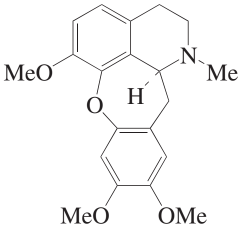


Baluchistanamine

Like the bisbenzylisoquinoline precursors, these alkaloids differ in the number and position of the diphenyl ether linkages. Karakoramine has only one such bond, Baluchistanamine has two, and Punjabine has three. **Secantioquine** and **Secolucidine** are examples of a biphenyl system.

CULARINE ALKALOIDS (VX2440)

The cularines are tetracyclic isoquinoline alkaloids which contain a dihydrooxepine or oxepine ring between *C*-8 and *C*-2′. They are formed by intramolecular oxidative coupling of 7,8,3′,4- or 7,8,4′,5′-tetraoxygenated tetrahydrobenzylisoquinolines (classical cularines and isocularines, respectively), although the biogenesis of **Gouregine** probably proceeds via oxidation of an aporphine precursor. Note the parallelism between the cularine and aporphine alkaloids.



Cularine

A small number of **Cancentrine**-type alkaloids are known which are cularine-morphinan dimers.

Castedo, L. *et al., Alkaloids*, 1986, **29**, 287–324 (*rev*)

SECOCULARINE ALKALOIDS (VX2450)

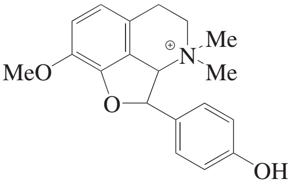
The secocularines can be divided into two sub-groups, namely B- and C-ring seco compounds. B-Ring secocularines, exemplified by **Secocularidine**, are structurally related to phenanthrene alkaloids derived from aporphines and are probably formed *in vivo* by Hofmann degradation of cularines. C-Ring cularines, represented by **Noyaine**, constitute a type of alkaloid without counterpart among aporphinoids.

INDENOBENZAZEPINE ALKALOIDS (VX2500)

This is a small group, e.g. **Lahorine,** which may be derived from the spirobenzylisoquinolines (VX3220 below).

QUETTAMINE ALKALOIDS (VX2470)

Whereas the classical-type cularine alkaloids of the Fumariaceae are biogenetically derived from intramolecular oxidative coupling of tetraoxygenated tetrahydroisoquinoline precursors, the quettamines are obtained from *in vivo* intramolecular oxidation of a trioxygenated tetrahydroisoquinoline. So far, few naturally occurring quettamines are known. These alkaloids, all found in *Berberis baluchistanica*, incorporate either a benzofuran or a dihydrobenzofuran ring within the molecular framework, and the seco bases possess an *N*,*N*-dimethylaminoethyl substituent.



Quettamine

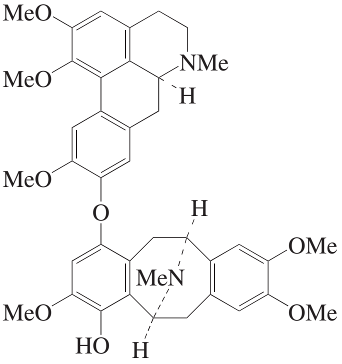
DIBENZOPYRROCOLINE ALKALOIDS (VX2480)

These alkaloids, only a few of which are known, are clearly derived by oxidation of a benzylisoquinoline precursor; indeed, the ring system was prepared *in vitro* by this route before it was encountered in nature. **Oubatchensine** is a 7,13-seco alkaloid presumably derived through 13-hydroxylation and tautomerism to the open-chain form.

Elliot, I.W., *Alkaloids*, 1987, **31**, 101–117 (*rev*)

PAVINE AND ISOPAVINE ALKALOIDS (VX2520, VX2540)

These alkaloids are formed by alternative modes of oxidative cyclisation of benzylisoquinoline precursors. In addition there are bisbenzylisoquinoline alkaloids composed of pavine and aporphine units, e.g. **Pennsylpavine**.



Pennsylpavine

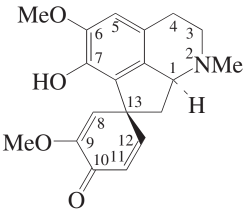
Because of the two-fold rotational symmetry of the pavane skeleton, there are numerous variations in numbering schemes in the literature. Numbering in this Dictionary has been regularised according to IUPAC principles.

Some mixed pavinoid-benzylisoquinoline and pavinoid-aporphine dimers (**Hervelines**, **Fauripavine**) have been isolated relatively recently.

Gözler, B. *et al., Alkaloids*, 1987, **31**, 317–390 (*rev*)

PROAPORPHINE ALKALOIDS (VX2600)

This group of alkaloids, e.g. **Orientalinone**, represents an intermediate stage in the conversion of the benzylisoquinoline alkaloids by phenol oxidative coupling into the aporphines. The spirocyclohexenone ring may occur in various oxidation levels from cyclohexadienone to cyclohexanol. There are various numbering schemes in the literature. That shown has been adopted here as standard.



Orientalinone

There are also proaporphine-tryptamine dimers centred on **Roehybridine**. These heptacyclic alkaloids, found in *Roemeria hybrid* (Papaveraceae) and *Phoebe grandis* (Lauraceae), are probably derived biogenetically by a Mannich-type condensation of a ketonic tetrahydroproaporphine with a tryptamine analogue.

PROAPORPHINE-BENZYLISOQUINOLINE ALKALOID DIMERS (VX2620)

This group is self-explanatory, e.g. **Pakistanamine**.

APORPHINE ALKALOIDS (VX2640, VX2700)

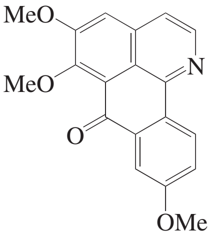
This large group of alkaloids contains the tetracyclic ring system formed by the phenol oxidative coupling of a benzylisoquinoline precursor. The structural variations among the numerous simple aporphines (VX2640) are mostly 6*a*,7-dehydrogenation and 7-oxidation, accompanied by isoquinoline-ring aromatisation in the so-called oxoaporphines, e.g. **Liriodenine** (VX2640). To this listing must be added a small group of bisaporphines. The majority of these alkaloids possess a carbon-to-carbon linkage between *C*-7 and *C*-7′ (e.g. **Urabaine**), although examples of C-C coupled bisaporphines and oxygen-bonded dimers (e.g. **Dehatriphine**) are also known. There is a considerable number of aporphine-benzylisoquinoline dimers listed separately (VX2700).

Various alkaloid groups which follow (VX2750-VX2840) may be considered as closely related to the true aporphines and are often reviewed alongside them.

Guinaudeau, H. *et al.*, *Lloydia*, 1975, **38**, 275–338; *J. Nat. Prod.*, 1979, **42**, 133–149, 325–360; 1983, **46**, 761–835; 1984, **47**, 565–580; 1988, **51**, 389–474, 1025–1053; 1994, **57**, 1033–1135 (*tabulations*)
Shamma, M., *Nat. Prod. Rep.*, 1986, **3**, 345–352 (*rev*)
Gözler, B. *et al.*, *J. Nat. Prod.*, 1990, **53**, 675–685 (*aporphine dimers*)

OXOISOAPORPHINES (VX2750)

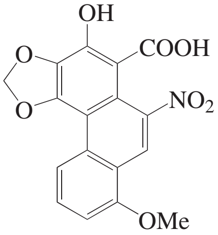
This is a small group of alkaloids, mostly from *Menispermum* spp. It has been suggested that they arise from aporphines via a spirodienone rearrangement, however, biosynthetic studies have not been reported. One of its representatives is **Menisporphine**. **Lakshminine**, from *Sciadoteria* sp., in the Menispermaceae, contains an additional nitrogen substituent.



Menisporphine

ARISTOLOCHIC ACIDS AND ARISTOLACTAMS (VX2780, VX2800)

The aristolochic acids represent a class of phenanthrenoid alkaloid derived from an aporphinoid precursor with ring-B fission and the loss of *C*-5 (aporphine numbering). **Aristolochic acid VIa** is a typical alkaloid. Some of the alkaloids are esters of these acids with, for example, terpenoids, e.g. **Aristolin**. They are higher plant products characteristic of the Aristolochiaceae. Since they have a seco-aporphinoid skeleton, they have been numbered in the literature in different ways, either as aporphines or as phenanthrenes, and for many of them (such as those with a methylenedioxy function), the CAS systematic numbering is different again. In this Dictionary, the simpler members are named and numbered as substituted phenanthrenes, and different alkaloid groups are collected into entries under the parent phenanthrene.



Aristolochic acid VIa

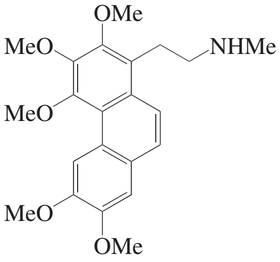
The biosynthetically-related Aristolactams, mostly nonbasic, have a five-membered lactam ring e.g. **Cepharanone A**.

These classes of alkaloid also include some members in which nitrogen has been oxidised to a nitro group, e.g. **Aristolochic acid A**.

Bick, I.R.C. *et al., Alkaloids*, 1985, **24**, 113–152 (*rev*)
Chen, Z., *Alkaloids*, 1987, **31**, 29–66 (*rev*)
Kumar, V. *et al.*, *Nat. Prod. Rep.*, 2003, **20**, 565–583 (*rev*)

PHENANTHRENE ALKALOIDS (VX2820)

These alkaloids, e.g. **Thalicpureine**, are related to aporphines by fission of the *N*-6*a* bond. The group includes a few alkaloids showing oxidative changes elsewhere in the molecule (**Andesine**; **Chiloenine**; **Santiagonamine**). **Eupolauramine** is related by a further ring-contraction to a lactam.

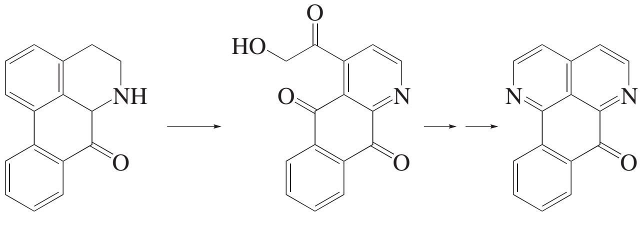


Thalicpureine

Taylor, W.C., *Aust. J. Chem.,* 1984, 37, 1095–1104 (*biosynth*)
Castedo, L. *et al., Alkaloids*, 1990, **39**, 99–138 (*rev*)

AZAAPORPHINE ALKALOIDS (VX2830)

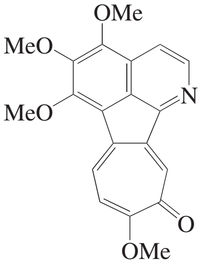
This fairly small group, e.g. **Sampangine**, is thought to arise by A-ring fission of an aporphinoid precursor to an azaanthraquinone intermediate, followed by ring closure.



Sampangine

AZAFLUORANTHENE ALKALOIDS (VX2840)

This is another small group of alkaloids found in the Menispermaceae. Two biosynthetic mechanisms have been proposed; cyclisation of a 1-arylisoquinoline (which is considered unlikely since 1-arylisoquinolines are rare) or a more persuasive route involving the decarbonylation of an oxoaporphine. **Imerubrine** and its relatives are then related by an aryl→tropolone expansion. **Eupolauridine** could arise by a combination of this route and the aza-replacement shown above under VX2830.

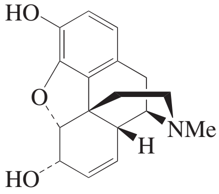


Imerubrine

Buck, K.T., *Alkaloids*, 1984, **23**, 301–327 (*rev*)
Taylor, W.C., *Aust. J. Chem.*, 1984, 37, 1095–1104 (*biosynth*)

MORPHINE ALKALOIDS (VX2900)

This extremely important group is formed by phenol oxidative coupling of a hydroxylated benzylisoquinoline precursor such as Norlaudanosoline, itself originating from two molecules of tyrosine. The group may be subdivided into bases of the **Salutaridine** type, those related to **Morphine**, which have a 4,5-oxide bridge, and those related to **Sinoacutine**, which are enantiomeric with the salutaridine group. **Acutumine** and its congeners represent an *abeo* shift to a spiro skeleton.

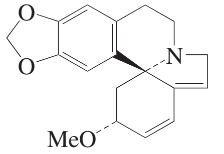


Morphine

Szantay, C. *et al., Alkaloids*, 1994, **45**, 128–232 (*rev*)

Erythrina alkaloids (VX2940)

This group of alkaloids is derived from two tyrosine units by oxidative coupling and intramolecular rearrangement. Alkaloids which contain the erythrinan skeleton (e.g. **Erythraline**) constitute the majority.



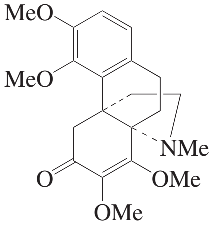
Erythraline

Major structural variations consist of oxidative modification of the aromatic ring to a lactone, e.g. **β-Erythroidine**, and a small group containing an additional nitrogen atom in ring D. These 16-azaerythrinanes, e.g. **Erymelanthine**, are possibly derived biogenetically by *in vivo* oxidation of the aromatic ring, followed by nitrogen uptake and recyclisation. There are also a few so-called dimeric alkaloids that incorporate a tryptophan moiety, e.g. **Erysopinophorine**.

Dyke, S.F. *et al., Alkaloids*, 1981, **18**, 1
Chawla, A.S. *et al., Alkaloids Chem. Biol. Perspect.,* 1991, **9**, 85–154 (*rev*)
Amer, M.E. *et al., J. Nat. Prod.*, 1991, **54**, 329–363 (*rev*)
Tsuda, Y. *et al., Alkaloids*, 1996, **48**, 249–337 (*rev*)

Dibenzazecine and hasubanan alkaloids (VX2980, VX3000)

These two groups may appear at first sight to belong to quite different structural groups, but there is little doubt that biosynthetically they are related. Both groups are derived from two tyrosine units, but their biosynthesis is not simple. A pivotal intermediate appears to be a hydroxylated benzylisoquinoline which can cyclise, by alternative phenol oxidative coupling processes, to a hydroxysalutaridine, or its isomer. This biosynthetic route is exceptional since it would appear that two hydroxy-groups need to be present in one of the aromatic rings. In all other known cases of oxidative coupling, only one hydroxy-group seems to be essential. The biosynthesis has affinities with that of the morphine alkaloids, although there is clearly an important divergence in the later stages.

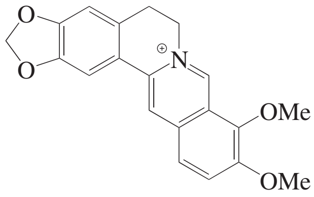


Hasubanonine

Inubushi, Y. *et al., Alkaloids*, 1977, **16**, 393–340 (*Hasubanans, rev*)
Matsui, M., *Alkaloids*, 1988, **33**, 307–347 (*Hasubanans, rev*)

PROTOBERBERINE ALKALOIDS (VX3100, VX3240)

These tetracyclic alkaloids are derived from benzylisoquinolines by condensation with a one-carbon unit (the berberine bridge), the additional carbon atom coming from the methionine-derived C_1 pool. The alkaloids most closely related to benzylisoquinolines are the simple tetrahydroprotoberberines, e.g. **Tetrahydropalmatine**, which are dehydrogenated to Protoberberines, such as **Berberine**. There are also alkaloids carrying extra carbon substituents at *C*-12 and *C*-13 such as **Orientalidine** and **Corydaline**, respectively, and ring-opened protoberberines (secoberberines) which can be regarded as benzylisoquinolines with a carbon substituent at *C*-2′. The latter may occur in different oxidation states: as an aldehyde (e.g. **Aobamine**), an alcohol (e.g. **Macrantaline**) or as a carboxylic acid (e.g. **Macrantoridine**).



Berberine

Structure determination in this series, i.e. the assignment of correct regiochemistry to the substituents on the protoberberine ring system, has been a matter of some difficulty in the past and it is possible that some of the current assignments will prove to be incorrect.

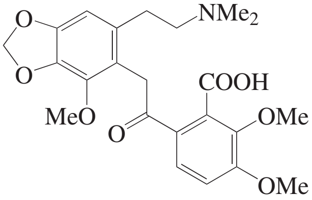
Jeffs, P.W., *Alkaloids*, 1967, **9,** 41–115 (*rev*)
Santavy, F., *Alkaloids*, 1979, **17**, 439–461 (*rev*)
Bhakuni, D.S. *et al., Alkaloids*, 1986, **28**, 95–181 (*rev*)
Beecher, C.W.W. *et al., Alkaloids Chem. Biol. Perspect.,* 1988, **6**, 297–337 (*rev*)
Leitao da Cunha, E.V. *et al., Alkaloids*, 2005, **62**, 1–75 (*rev*)
Grycova, L. *et al., Phytochemistry*, 2007, **68**, 150–175 (*rev*)

ISOINDOLOBENZAZEPINE ALKALOIDS (VX3130)

This is a small group, one example is **Lennoxamine**, which is a popular synthetic target.

NARCEINE ALKALOIDS (VX3140)

These alkaloids constitute further examples of oxidation products of protoberberines, in which the nitrogen to *C*-8 bond has been cleaved. The narceine group contain an ethanamine chain and, as well as relatives of **Narceine**, include bases which contain an enol lactone function, and those with a higher (**Bicucullinine**) or lower (**Peshawarine**) oxidation level than **Narceine**.

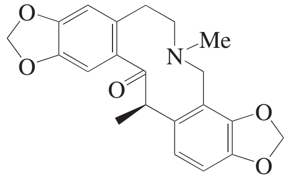


Narceine

Blaskó, G. *et al.*, *J. Nat. Prod.*, 1982, **45**, 105–122 (*rev*)

PROTOPINE ALKALOIDS (VX3160)

These tricyclic bases are simply formed by oxidative ring fission of protoberberine *N*-metho salts. Two of these bases (**Corycavamine**, **Corycavidine**) have an additional methyl group at *C*-13.

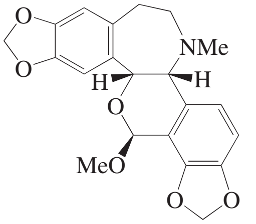


Corycavamine

Guinaudeau, H. *et al.*, *J. Nat. Prod.*, 1982, **45**, 237–246 (*rev*)
Onda, M. *et al., Alkaloids*, 1988, **34**, 181–209 (*rev*)

RHOEADINE ALKALOIDS (VX3180)

This group of alkaloids has been encountered only in *Papaver* and related genera. Their biogenesis appears to be from two tyrosine units, via tetrahydroberberine and protopine intermediates. Oxidative fission of the nitrogen to *C*-8 bond followed by oxidative cyclisation of nitrogen on to *C*-15 and lactol formation results in a ring system in which *C*-8 becomes the lactol carbon atom.



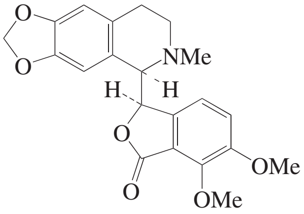
Rhoeadine

CAS formerly employed the semisystematic skeleton Rheadan for naming these alkaloids, but this has been abandoned in favour of systematic nomenclature (Rheadan = [2]Benzopyrano[3,4-*a*][3]benzazepine).

Rönsch, H., *Alkaloids*, 1986, **28**, 1–94 (*rev*)

PHTHALIDEISOQUINOLINE ALKALOIDS (VX3200)

These are closely related to the rhoeadine group, and like them are formed in nature by oxidation of tetrahydroprotoberberines; **Hydrastine** and **Narcotine** are specifically derived from Reticuline via Scoulerine.

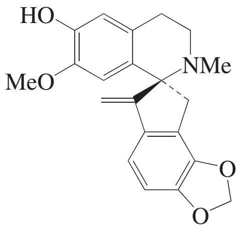


Hydrastine

MacLean, D.B., *Alkaloids*, 1985, **24**, 253–286 (*rev*)

SPIROBENZYLISOQUINOLINE ALKALOIDS (VX3220)

These alkaloids are derived from protoberberines by a 1,2-shift of *C*-8 from nitrogen to *C*-14. Several mechanisms are possible, but since several of the alkaloids contain oxygen at *C*-13 a route through an enolate ylid is attractive. **Ochotensine** and its relatives contain an additional carbon atom, again derived from methionine. Closely related to this group is **Lahorine**, an indenobenzazepine derivative, which may be derived biogenetically from the spirobenzylisoquinolines. **Hyperectine** represents a unique type of alkaloid substituted with an imidazole group.



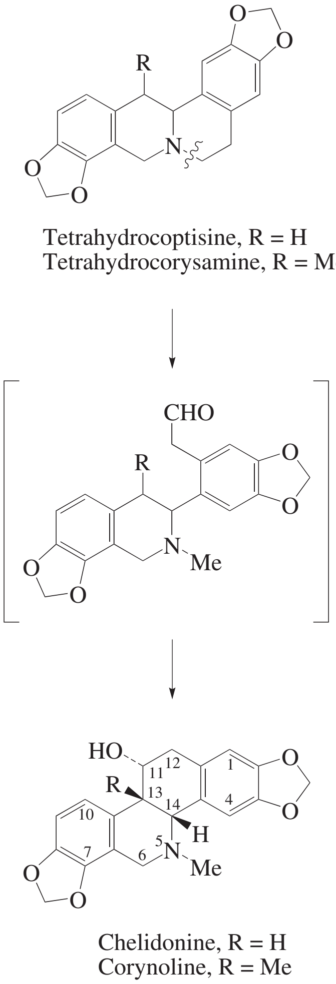
Ochotensine

Presiner, R.M. *et al.*, *J. Nat. Prod.*, 1980, **43**, 305–318 (*rev*)

Benzo[*c*]phenanthridine alkaloids (VX3300)

These alkaloids are derived from tetrahydroprotoberberine precursors by oxidative cleavage of the *C*-6 to nitrogen bond, followed by cyclisation of *C*-6 on to position 13. Various oxidation stages exist, e.g. partially reduced benzophenanthridines, as in **Chelidonine**, and fully aromatic systems, as in **Sanguinarine**. There are also secoalkaloids (**Arnottianamide**), dimers, e.g. **Sanguidimerine**, and a group formed by the addition of a carbon substituent to *C*-8 e.g. **Corynolamine**, which in some alkaloids has undergone further elaboration (**Buesgeniine**, **Chelelactam**, **Nitrotyrasanguinarine**).

Several numbering systems have been used for the benzophenanthridine alkaloids, but the one shown below, based on biogenetic considerations, has been adopted in this Dictionary (this is not the numbering scheme for Benzo[*c*]phenanthridine itself).



Tetrahydrocoptisine, R = H
Tetrahydrocorysamine, R = Me

Chelidonine, R = H
Corynoline, R = Me

Simanek, V., *Alkaloids*, 1985, **26**, 185–240 (*rev*)
Iwasa, K. *et al., J.A.C.S.*, 1989, **111**, 7925–7931 (*biosynth*)

PHENETHYLISOQUINOLINE ALKALOIDS (VX3360)

This group (e.g. **Autumnaline**) arises from a phenethylisoquinoline precursor, which is itself generated by condensation of tyrosine with a C_6-C_3 unit derived from phenylalanine, probably via cinnamic acid.

In addition to the small group of simple phenethylisoquinolines (including dimers; **Jolantinine**; **Melanthioidine**), several other members of the following groups are related to them by further elaboration.

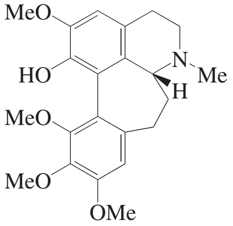
Kametani, T. *et al., Alkaloids*, 1973, **14**, 265–323; 1989, **36**, 172–223 (*revs*)

HOMOMORPHINANDIEONE ALKALOIDS (VX3370)

This is a small group, e.g. **Androcymbine**, which are biosynthetic intermediates between the phenethylisoquinolines and the colchicines (VX3400). Androcymbine arises by phenol oxidative coupling, probably of Autumnaline, by a process analogous to that involved in the biosynthesis of the morphine alkaloids.

HOMOAPORPHINE AND HOMOPROAPORPHINE ALKALOIDS (VX3380, VX3390)

The sequence from tyrosine and phenylalanine through a phenethylisoquinoline to the homoproaporphines and homoaporphines appears superficially to be exactly analogous to the course of biosynthesis of the aporphine alkaloids. However, although Autumnaline (VX3360 above) is an efficient precursor for both **Kreysiginone** and **Kreysigine** in *Kreysigia multiflora*, dienone intermediates such as Kreysiginone are not involved in the biosynthesis of the homoaporphines, such as Kreysigine. **Bitlisine** represents an anomalous type.

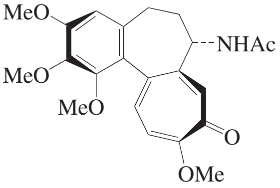


(-)-Kreysigine

Tojo, E., *J. Nat. Prod.*, 1989, **52**, 909–921 (*listing*)

COLCHICINE ALKALOIDS (VX3400)

Autumnaline (VX3360) and *O*-Methylandrocymbine (VX3370) (but not Androcymbine itself) are efficient precursors for **Colchicine**, an important pharmaceutical and research tool, and the details of the biosynthesis have been studied in detail.



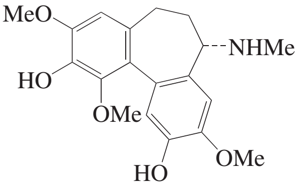
Colchicine

Lumicolchicines are the product of u.v. irradiation of Colchicine, and while they have been reported to occur naturally, they could be regarded as artifacts. The rearrangement product **Demecolcinone** has also been isolated more recently.

Capraro, H.-G. *et al., Alkaloids*, 1984, **23**, 1–72 (*rev*)
Boyè, O. *et al., Alkaloids*, 1992, **41**, 125–176 *(rev)*
Battersby, A.R. *et al., J. Chem. Soc., Perkin Trans. 1*, 1998, 2989–2994; 2995–3001; 3002–3009 (*biosynth*)
Le Hello, C., *Alkaloids*, 2000, **53**, 287–352 (*pharmacol*)

DIBENZOCYCLOHEPTYLAMINE ALKALOIDS (VX3410)

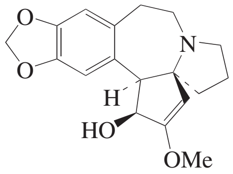
Dibenzocycloheptylamine alkaloids are found in plants of the genera *Colchicum* and *Androcymbium*. To date only a few are known; these include **Jerusalemine** and **Salimine**. Jerusalemine may be formed through decarbonylation of the tropolone ring of 2-Demethyldemecolcine by a peroxidase system present in the plant, with accompanying oxidation. Salimine, on the other hand, may arise from Colchicine by enzymatic peroxidation of ring C followed by hydroxylation and methylation.



Jerusalemine

CEPHALOTAXUS ALKALOIDS (VX3420)

A group of alkaloids from *Cephalotaxus* spp. (Cephalotaxaceae) in which the hydroaromatic component of the Erythrina group (VX2940 above) has undergone skeletal rearrangement. A typical alkaloid of this group is **Cephalotaxine**. Alkaloids occur in both enantiomeric series and some are potent antitumour agents.

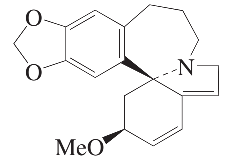


Cephalotaxine

Huang, L., *Alkaloids*, 1984, **23**, 157–227 (*rev*)
Miah, M.A.J., *Alkaloids*, 1998, **51**, 199–269 (*rev*)

HOMOERYTHRINA ALKALOIDS (VX3440)

E.g. **Schelhammeridine**. These would appear to be formed by a route analogous to that adopted in the Erythrina group (VX2940). **Selaginoidine** and **Phellibiline** represent unusual types involving oxidative degradation of the aryl ring.



Schelhammeridine

Bick, I.R.C. al, Alkaloids Chem. Biol. Perspect., 1989, **7**, 1–42 (rev)

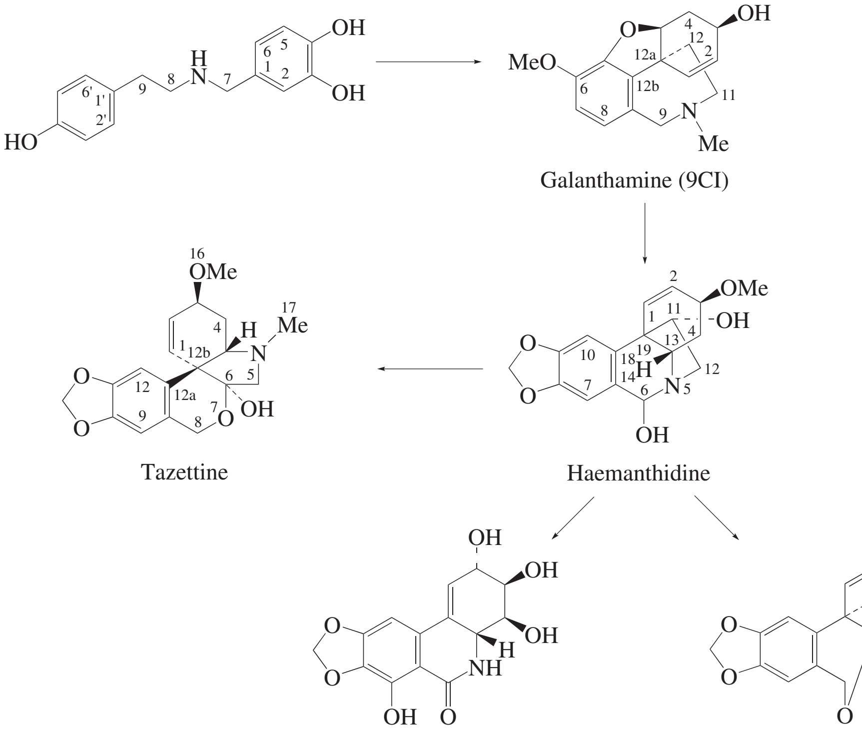
AMARYLLIDACEAE (NARCISSUS) ALKALOIDS (VX3510-VX3599)

This large group of alkaloids is also derived from two tyrosine units which combine, with loss of one carbon atom, to give a benzylphenylethylamine precursor unit, e.g. **Norbelladine**. Various oxidative cyclisation processes, prominent among which are phenol oxidative coupling reactions, can give rise to the major skeletal groups. The unprimed aromatic ring derives from a simple aromatic precursor such as vanillin.

Oxidation of a norbelladine-type precursor at *C*-7, followed by cyclisation at *C*-2′, gives the simple 1-aryltetrahydroisoquinolines (VX3510) exemplified by **Cryptostylines I** and **II**. Some representatives are also found in the Orchidaceae; and both enantiomers of Cryptostyline and of some other Amaryllidaceae alkaloids have been isolated from different plants. Oxidation at the alternative benzylic position (*C*-9) and cyclisation at *C*-6 gives the 4-aryltetrahydroisoquinolines related to **Cherylline** (VX3520). Some 4- aryltetrahydroquinolines (e.g. **Viridicatin**) have been isolated from microorganisms. Oxidative coupling of positions 2 and 2′ gives the apogalanthamine skeleton of **Nivalidine** (VX3530), although this may be an artifact derived from Galanthamine.

Oxidative coupling of *C*-2 with *C*-1′ in Norbelladine gives the **Galanthamine** (VX3540) skeleton which, by a straightforward cyclisation process (nitrogen to position 1), can give rise to the **Haemanthidine** (VX3550) ring system. The more recently discovered **Graciline** subgroup (VX3555) is related to Haemanthidine by *N*(5)-*C*(6) fission and pyran ring formation.

Opening of the carbinolamine function in Haemanthidine, followed by a redox reaction and cyclisation of the oxygen at *C*-6 on to position 11 (Haemanthidine numbering), then affords the **Tazettine** (VX3560) skeleton.



Galanthamine (9CI)

Tazettine

Haemanthidine

Narciclasine

Graciline

A further possibility is the migration of *C*-18 in the haemanthidine skeleton to position 11, which gives rise to the ring systems present in **Pancracine** (VX3570) type alkaloids.

A double cyclisation of *C*-2 to *C*-3′ and nitrogen to *C*-2′ provides the tetracyclic skeleton characteristic of **Lycorine** and its analogues (VX3580). Further modification of this ring system by oxidative fission of the nitrogen to *C*-7 bond followed by attachment of oxygen at *C*-7 to position 1 (galanthan numbering) then gives rise to the **Lycorenine** group (VX3585). A small number of Lycorenine alkaloids exemplified by **Galanthindole** show aromatisation of the indole portion, leading to a type of non-tryptophan-derived, biogenetically distinct type of indole alkaloid.

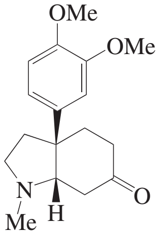
The small **Narciclasine** group (VX3590) also stems from Norbelladine, and appears to be formed via Crinine (but not 3-Epicrinine) by loss of the two-carbon bridge and appropriate oxidations.

Category VX3599, Miscellaneous Amaryllidaceae alkaloids, includes **Ismine**, an aromatised biaryl derived from a Haemanthidine precursor, and some novel two-nitrogen alkaloids such as **Plicamine**, and **Augustamine**, which cannot be assigned to known subtypes. There also remain a considerable number of alkaloids from earlier work to which structures were not assigned. **Varadine**, isolated in 1979, deserves reinvestigation.

Martin, S.F., *Alkaloids*, 1987, **30**, 252–369 (*rev*)
Hoshino, O., *Alkaloids*, 1998, **51**, 323–424 (*rev*)
Prabhakar, S. *et al., Alkaloids Chem. Biol. Perspect.*, 2001, **15**, 433–572 (*rev, synth*)
Bastida, J. *et al., Alkaloids*, 2006, **63**, 87–179 (*rev*)
Jin, Z., *Nat. Prod. Rep.*, 2007, **24**, 886–905 (*rev*)
Unver, N., *Phytochem. Rev.*, 2007, **6**, 125–135 (*rev, new types of Amaryllidaceae alkaloid*)

MESEMBRENOID ALKALOIDS (VX3600)

Derived from two phenylalanine units with loss of one of the ethanamine sidechains, this smallish group of alkaloids is typified by **Mesembrine**; a second sub-group contains alkaloids in which the pyrrolidine ring has not been formed, as in **Joubertiamine**. A third variant contains bases in which a pyridine ring has been fused on, as in **Sceletium alkaloid A4** and **Tortuosamine.** Mesembrenoid alkaloids occur in *Sceletium* spp. (Aïzoaceae).

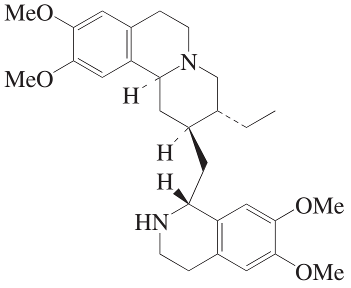


Mesembrine

Jeffs, P.W. *et al., Alkaloids,* 1981, **19**, 1–80 (*rev*)
Jin, Z., *Nat. Prod. Rep.*, 2007, **24**, 886–905 (*rev*)

Emetine (Ipecac) alkaloids (VX3690)

The emetine alkaloids are unique among the isoquinoline group in that they are derived from a monoterpenoid unit via Secologanin in an analogous manner to the monoterpenoid indole alkaloids. They occur in the Alangiaceae, Rubiaceae and Icacinaceae. Incorporation of one phenylalanine/tyrosine unit gives the alkaloids exemplified by **Ipecoside** and **Protoemetine**; the latter, by combination with a second amino acid unit, gives rise to the **Emetine** subgroup. Alternatively, combination with a tryptamine unit gives the typical alkaloids of *Alangium lamarckii,* e.g. **Tubulosine**.

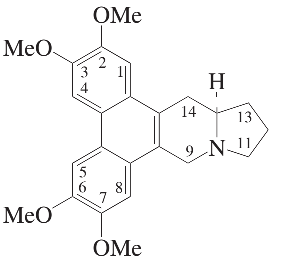


Emetine

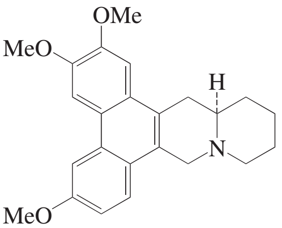
Fujii, T.M. *et al., Alkaloids*, 1983, **22**, 1–50; 1998, **51**, 271–321 (*revs*)
Wiegrebe, W. *et al.*, *J. Nat. Prod.*, 1984, **47**, 397–408 (*rev*)

Phenanthroindolizidine and phenanthroquinolizidine alkaloids (VX3700, VX3760)

These alkaloids are derived from two molecules of phenylalanine or tyrosine, together with, presumably, ornithine (phenanthroindolizidines. e.g. **Tylophorine**) or lysine (phenanthroquinolizidines, e.g. **Cryptopleurine**).



Tylophorine

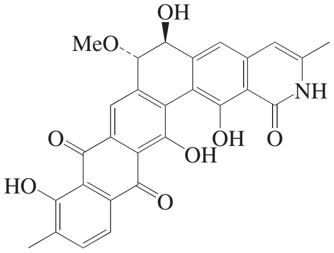


Cryptopleurine

Bick, I.R.C. *et al., Alkaloids*, 1981, **19**, 193–220 (*rev*)
Gellert, E. *et al., Alkaloids Chem. Biol. Perspect.,* 1987, **5**, 55–132 (*rev*)
Michael, J.P., *Nat. Prod. Rep.*, 2004, **21**, 625–649; 2005, **22**, 603–626; 2008, **25**, 139–165 (*revs*)

ERICAMYCINS (VX3900)

This is a relatively small group of polycyclic substances containing a fused isoquinoline system which has been little reviewed. The name Ericamycins is used here; although they are also referred to as the Albofungin group. They are of polyketide origin, with some unusual features to their biosynthesis. Various numbering systems have been used, and the numbering in CAS changes for trivial reasons (presence or absence of additional alicyclic rings, etc.)



Ericamycin

Bockholt, H. *et al., J. Org. Chem.*, 1994, **59**, 2064–2069 (*biosynth*)

INDOLE ALKALOIDS

The group of alkaloids derived from tryptophan constitutes the largest, most varied and most fascinating of all alkaloid groups. The alkaloids include simple tryptamine derivatives, carbazoles (in which the ethanamine chain has been lost), a variety of alkaloids in which tryptamine has combined with one or more prenyl residues, and others in which regular monoterpenoid or diterpenoid units have been incorporated. However, the largest group, and the most extensively studied, is the thousands of alkaloids derived from tryptophan and a monoterpenoid unit based on Secologanin. The classical researches on indole alkaloids were carried out on terrestrial plant alkaloids, and then moved to studies of fungal-derived alkaloids. Indole alkaloids are also numerous in marine organisms, and the range of structural types differs from those found in terrestrial organisms. Many of the 'traditional' indole alkaloid types produced by terrestrial plants have not been found; polyhalogenation is a common feature of these alkaloids.

SIMPLE INDOLE ALKALOIDS (VX4000)

Under this heading appear various unhalogenated (plant) and halogenated (marine) indoles, together with higher molecular weight alkaloids containing unsubstituted indole ring systems, such as **Aplysinopsin** and its relatives (which are also imidazoles). Also included are a variety of simple indoles carrying prenyl, etc. substituents. The simplest plant indole alkaloid is **Gramine**.

Husson, H.-P., *Alkaloids*, 1985, **26**, 1–51 (*rev*)
Higuchi, K. *et al.*, *Nat. Prod. Rep.*, 2007, **24**, 843–865 (*rev*)

BISINDOLES (VX4020)

This category includes **Indirubin**, **6,6′-Dibromoindigotin** and other bisindoles; many from marine sources are polybrominated.

Yang, C.G. *et al., Curr. Org. Chem.*, 2004, **8**, 1691–1720 (*rev, bisindole alkaloids from sponges*)
Kam, T.-S. *et al., Alkaloids,* 2006, **63**, 181–337 (*rev*)

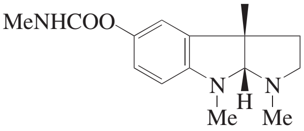
SIMPLE TRYPTAMINE ALKALOIDS (VX4040)

Tryptamine itself and some simple relatives have been isolated from marine tissues, and **Bufotenine**, long known as an amphibian product, has more recently been detected in a gorgonian. More highly elaborated marine alkaloids containing a (dehydro)tryptamine residue include the **Kottamides**. There are also some simple tryptamine dimers and oligomers such as the **Gelliusines**.

Somei, M. *et al.*, *Nat. Prod. Rep.*, 2004, **21**, 278–311 (*rev*)
Kawasaki, T. *et al.*, *Nat. Prod. Rep.*, 2005, **22**, 761–793 (*rev*)
Kam, T.-S. *et al., Alkaloids,* 2006, **63**, 181–337 (*rev*)

CYCLOTRYPTAMINE ALKALOIDS (VX4100)

This group is formally derived from tryptophan by cyclisation and decarboxylation. (The presence of the cyclised form, cyclotryptophan, can be demonstrated in tryptophan solutions). **Physostigmine**, the prototype of this group of alkaloids, was first isolated from *Physostigma venenosum* and has also been produced by *Streptomyces* spp. The alkaloid is characterised by a urethane group which is readily hydrolysed with aqueous base to afford Eseroline. In addition to plant alkaloids with this skeleton, other representatives of this class have been isolated from marine organisms (e.g. the **Flustramines**) and from skin extracts of the Australian frog *Pseudophryne coriacea* (e.g. **Pseudophrynamine A**, where there is evidence for *de novo* biosynthesis by the amphibian rather than a dietary source). A number of interesting oligomers of this class occur in plants, e.g. **Chimonanthine**, a dimer, **Hodgkinsine** (a trimeric species), the **Quadrigemines** (tetramers) and higher.

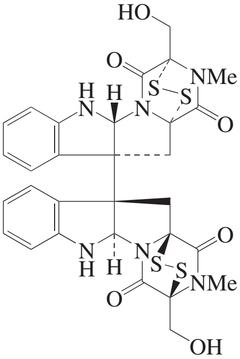


Physostigmine

Anthoni, U. *et al., Alkaloids Chem. Biol. Perspect.*, 1999, **13**, 163–236 (*rev*)
Kam, T.-S. *et al., Alkaloids,* 2006, **63**, 181–337 (*rev*)

CHAETOCIN ALKALOIDS (VX4110)

Also called Epipolythiodioxopiperazines, although some members of the series lack the polysulfur bridge. These are microbial products, but a considerable number, including the extensive series of **Leptosins**, have been isolated from marine sources. The prototype is **Echinulin**, from *Aspergillus echinulatus.* They are biosynthesised from diketopiperazines, which are cyclic amino acid anhydrides.

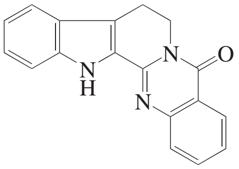


Chaetocin

Williams, R.M. *et al., Top. Curr. Chem.*, 2000, **209**, 97–173 (*prenylated tryptophans, biosynth*)
Somei, M. *et al., Nat. Prod. Rep.*, 2004, **21**, 278–311(*rev*)
Gardiner, D.M. *et al., Microbiology (Reading, U.K.)*, 2005, **151**, 1021–1032 (*biosynth*)
Kawasaki, T. *et al., Nat. Prod. Rep.*, 2005, **22**, 761–793 (*rev*)

EUODIA (QUINAZOLINOCARBAZOLE) ALKALOIDS (VX4120)

These alkaloids are characteristic of the Rutaceae. The most studied is **Rutaecarpine**, which has useful hypotensive activity. They arise by incorporation of a C_1 unit into a β-carboline precursor.

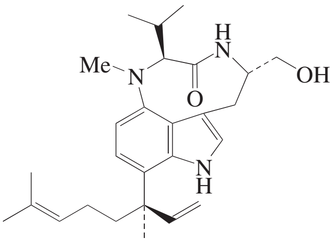


Rutaecarpine

Bergmann, J., *Alkaloids*, 1983, **21**, 29–55 (*rev*)

Indolactam alkaloids (VX4200)

The indolactam group contains an unusual nine-membered lactam ring derived from tryptophan and valine, via *N*-Methyl-L-isoleucyl-L-tryptophanol. The grouping occurs in the tumour-promoting **Teleocidins** and **Lyngbyatoxins**, which are microbial products. These contain a monoterpenoid portion which is derived from glucose, not mevalonate.

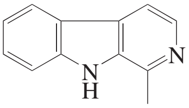


Lyngbyatoxin A

Irie, K *et al., Tet. Lett.*, 1990, **31**, 7337–7340; 1998, **39**, 7929–7930 (*biosynth*)

β-Carboline alkaloids (VX4240)

A large number of relatively simple β-carboline (pyrido[3,4-*b*]indole) derivatives occur naturally. These include β-carbolines unsubstituted at *C*-1, e.g. **1,2,3,4-Tetrahydro-6-methoxy-2-methyl-β-carboline**, those containing a methyl group at *C*-1, i.e. the **Harman** group, and several which contain a substituent at *C*-1 and/or *C*-3. The substituents at position 1 may be acyl, carboxyl, or they may be more complex, as in **Perlolyrine**



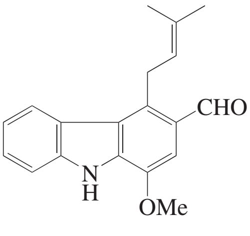
Harman

Long known as terrestrial alkaloids, these are also widespread in marine organisms. β-Carboline (**Norharman**) itself has been found in an ascidian and in dinoflagellates, and examples of simple brominated analogues include the **Eudistomins** and some of the **Arborescidines**. Another group of β-carboline derivatives, presumably derived from tryptophan and cysteine, have been isolated from *Eudistoma olivaceum*, a Caribbean tunicate. The β-Carboline nucleus is also found in some of the **Manzamines** and other more complex alkaloids.

Husson, H.-P., *Alkaloids*, 1985, **26**, 1–51 (*rev*)
Baker, B.J. *et al., Alkaloids Chem. Biol. Perspect.,* 1997, **10**, 357–407 (*rev, marine β-carbolines*)
Somei, M. *et al.*, *Nat. Prod. Rep.*, 2004, **21**, 278–311 (*rev*)
Fresneda, P.M. *et al.*, *Synlett*, 2004, 1–17 (*rev, synth*)
Kawasaki, T. *et al.*, *Nat. Prod. Rep.*, 2005, **22**, 761–793 (*rev*)

Carbazole alkaloids (VX4300)

Nearly all carbazole alkaloids have a substituent at *C*-3, although **Carbazole** itself and one or two simple marine halogenated derivatives have also been characterised. The main source of carbazole alkaloids are the plants of the Rutaceae subfamily Aurantioideae, especially the genera *Clausenia*, *Murraya* and *Glycosmis*. They are also found in some other higher plants, as well as streptomycetes and cyanobacteria. **3-Methylcarbazole** appears to be the key biosynthetic intermediate, although there is little direct experimental evidence. Elaboration into prenylcarbazoles (e.g. **Ekeberginine**) and dimerisation occurs. They have been well-reviewed.

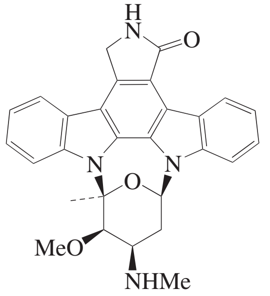


Ekeberginine

Husson, H.-P., *Alkaloids*, 1985, **26**, 1–51 (*rev*)
Chakraborty, D.P., *Alkaloids*, 1993, **44**, 257–364 (*rev*)
Knölker, H.-J. *et al.*, *Chem. Rev.*, 2002, **102**, 4303–4428 (*rev*)
Knölker, H.-J., *Curr. Org. Synth.*, 2004, **1**, 309–331 (*rev*, *synth*)
Somei, M. *et al.*, *Nat. Prod. Rep.*, 2004, **21**, 278–311 (*rev*)
Kawasaki, T. *et al.*, *Nat. Prod. Rep.*, 2005, **22**, 761–793 (*rev*)
Knölker, H.-J. *et al.*,, *Alkaloids*, 2008, **65**, 3–158; 159–180; 189–194; 195–384 (*occurrence*, *biosynth*, *biochem*, *chemistry*)

INDOLO[2,3-*A*]CARBAZOLE ALKALOIDS (VX4350)

These are a class of alkaloids exemplified by **Staurosporine**, which was first isolated in 1977 from a terrestrial microorganism, and which has since been found to be widely distributed. They are essentially microbial metabolites from a variety of organisms (field-collected or cultured), and show a wide range of biological activities. Others are the **Tjipanazoles** (from the blue-green alga *Tolypothrix tjipanasensis*) and several metabolites from slime moulds of the genus *Arcyria* (e.g. the **Arcyriarubins** and **Arcyriaflavins**). The isolation of **4′-*N,O*-Didemethylstaurosporine** from a flatworm *Pseudoceros* sp. is noteworthy. Their biosynthesis has been intensively studied; they are produced from bisindolyl precursors resembling **Violacein**; the indolyl residues are derived from tryptophan via 7-chlorotryptophan followed by an oxidative ring closure.

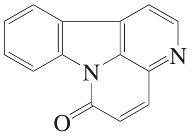


Staurosporine

Gribble, G.W. *et al.*, *Studies in Natural Product Chemistry*, (ed. Atta-ur-Rahman), Elsevier, 1993, **12**, 365 (*rev*)
Walsh, C.T. *et al.*, *Nat. Prod. Rep.*, 2006, **23**, 517–531 (*rev*, *biosynth*)
Sanchez, C. *et al.*, *Nat. Prod. Rep.*, 2006, **23**, 1007–1045 (*rev*, *biosynth*)

INDOLONAPHTHYRIDINE ALKALOIDS (VX4400)

These are the canthinones, a numerous and relatively straightforward subgroup of the β-carbolines, e.g. **Canthin-6-one**, in which an additional C_3 unit is attached between C-1 and the indole nitrogen to form an additional ring. The C-3 unit appears to be derived from ketoglutarate. The group includes a few dimeric examples, e.g. **Haplophytine**. They occur especially in the Simaroubaceae and Rutaceae, and some representatives have been isolated from basidiomycete fungi.



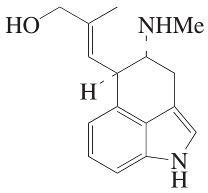
Canthin-6-one

Aragozzini, F. *et al., Plant Cell Rep.*, 1988**, 7**, 213–215 *(biosynth)*
Ohmoto, T. *et al., Alkaloids* 1989, **36**, 135–170 *(rev)*

ERGOT ALKALOIDS (VX4460)

These alkaloids, which classically occur in the fungus *Claviceps purpurea* which in the past was responsible for ergotism, are derived from 4-prenyltryptophan by cyclisation to give a tricyclic base related to **Chanoclavine I**, a representative of the simplest subgroup. Further elaboration gives the tetracyclic ergoline skeleton, as in

Elymoclavine, which is present in the majority of alkaloids in this group. The most important alkaloids, many of which have useful medical applications, are more complex peptide alkaloids formed from lysergic acid, in which *C*-17 in the elymoclavine-type precursor has been oxidised to a carboxyl group, by attachment to one or more amino acids. **Ergocristine**, which is based on the ergotaman nucleus, is typical.



Chanoclavine I

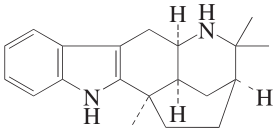
They have been considered exclusively the metabolites of terrestrial fungi and microorganisms, but the recent isolation of the **Pibocines**, simple brominated analogues of Festuclavine, from *Eudistoma ascidians*, have provided a first marine occurrence. The presence of the bromine substituent in the Pibocines argues for their being genuine ascidian products and this is presumably a case of biochemical parallelism.

A few other metabolites, which may also be included in this group, are the result of skeletal rearrangement. **Clavicipitic acid** is one such compound; another is **α-Cyclopiazonic acid**. However, whereas the former is definitely a product of prenyl-tryptophan metabolism the latter, from *Penicillium cyclopium* is not, since it appears to arise from reaction of a tryptophan-acetoacetate unit with prenyl pyrophosphate.

Floss, H.G., *Tetrahedron*, 1976, **32**, 873–912 (*rev*, *biosynth*)
Horwell, D.C., *Tetrahedron*, 1980, **36**, 3123–3149 (*rev*, *synth*)
Ergot Alkaloids: Chemistry, Biological Effects, Biotechnology, (eds. Řehaček, Z. *et al.*), Elsevier, 1990 (*rev*)
Groger, D. *et al., Alkaloids*, 1997, **50**, 171–218 (*rev*, *biochem*)
Somei, M. *et al., Alkaloids*, 2000, **54**, 191–257 (*rev*, *synth*)
Mukherjee, J. *et al., Biochem. Eng. Biotechnol.*, 2000, **68**, 1–20 (*rev*)
Schardl, C.L. *et al., Alkaloids*, 2006, **63**, 45–86 (*rev*, *biochem*)

INDOLOTERPENOID ALKALOIDS (VX4620)

This group consists of a variety of alkaloids in which a tryptamine unit is attached to a terpenoid unit. It includes the *Aristotelia* alkaloids, of which **Aristoteline** is typical, and some other terrestrial alkaloids isolated from *Borreria* spp. There are numerous variations in the structure of the terpenoid part of the skeleton. Also included here are the **Hapalindoles** and related alkaloids mostly from freshwater cyanophytes, which are mostly isocyano/isothiocyanato substituted.



Aristoteline

Alkaloids included in this classification code are not 'monoterpenoid indole alkaloids' in the strict sense as defined below for subsequent categories derived from secologanin. They are also distinguished in the classification code from the Penitrem group, VX6470.

Bick, I.R.C., *Alkaloids*, 1985, **24**, 113–151 (*rev*)
Borschberg, H.J., *Chimia*, 1991, **45**, 325–341 (*rev*)
Borschberg, H.J., *Alkaloids*, 1996, **48**, 190 (*rev*)

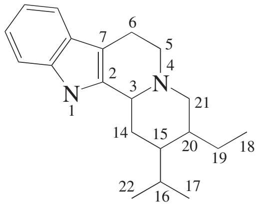
MONOTERPENOID-DERIVED INDOLE ALKALOIDS (VX4640-VX5980)

The extremely important and varied group of monoterpenoid indole alkaloids originate from the condensation of tryptophan with secologanin to give **Strictosidine**, which is further elaborated to give the corynanthe alkaloids, together with an impressive array of structural variants which are divided here into the numerous sub-groups tabulated in Table 1, and which are also described in the category descriptions which follow. Not all of the smaller groups of indole alkaloids are described in detail in the paragraphs which follow. If there is no description, their generic structure can be seen in Table 1, and any important references and reviews concerning them can be accessed from the individual dictionary entries.

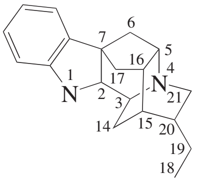
Various schemes have been used to divide the indole alkaloids into major groups based on the major biogenetic branch points. The most widely used recognises classes 1-5, where class 1 contains those skeletons most closely related to secologanin. These schemes are not further referred to in the discussion which follows. Certain biogenetic generalisations can be made, e.g. class 3 alkaloids are found only in the Apocynaceae.

Biogenetic numbering is used throughout this introduction and the individual entries. (Le Men, J.*, et al., Experientia*, 1965, **21**, 508–510; Anon., *Alkaloids*, 2001, **56**, xxiii–xxiv). This almost invariably differs from systematic (e.g. CAS) numbering. However, it allows the biogenetic origin of the individual carbons in the different types of indole alkaloid to be traced in the numerous skeletons. It does have the slight disadvantage that the numbering becomes discontinuous whenever there are new bond-making and bond-breaking processes, as illustrated in the chart. CAS numbering may be encountered for some groups, such as the Iboga alkaloids, but the Le Men biogenetic scheme is preferred by the majority of specialists in the field.

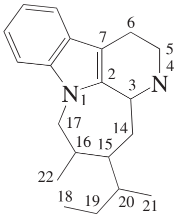
Table 1. Monoterpenoid indole alkaloid skeletons



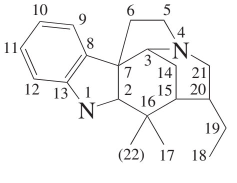
Ajmalicine skeleton
VX4860



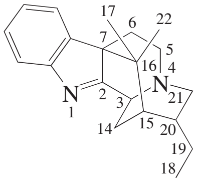
Ajmaline skeleton
VX5120



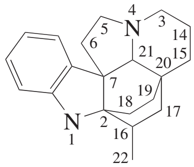
Akageran skeleton
VX4840



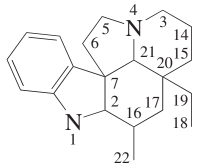
Akuammicine skeleton
VX5260



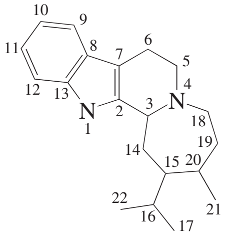
Akuammiline skeleton
VX5200



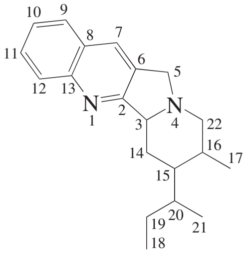
Aspidofractine skeleton
VX5540



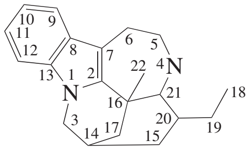
Aspidosperma skeleton
VX5400



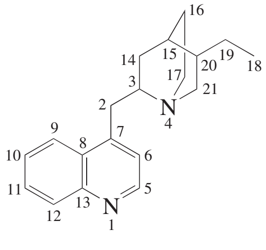
Cadamban skeleton
VX4940



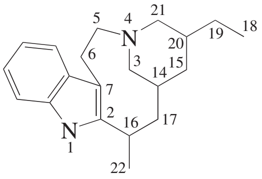
Camptothecin skeleton
VX4700



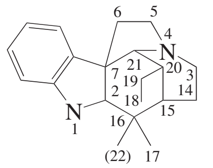
Chippiine skeleton
VX5940



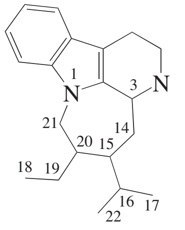
Cinchona skeleton
VX5240



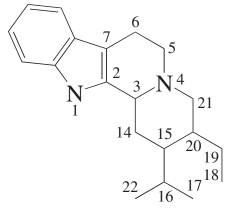
Cleavamine skeleton
VX5820



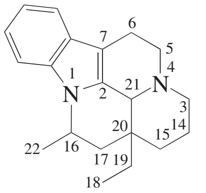
Condylocarpan skeleton
VX5320



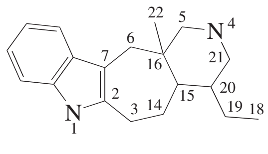
Correantan skeleton
VX4840



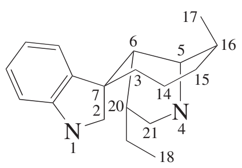
Corynanthean skeleton
VX4800



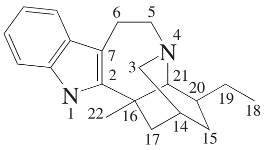
Eburna skeleton
VX5900



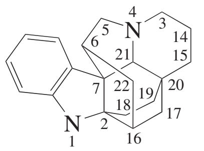
Ervatamia skeleton
VX5180



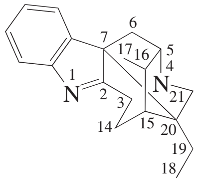
Gelsemium skeleton
VX5000



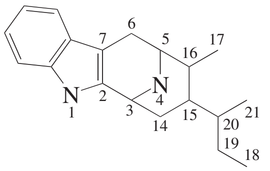
Iboga skeleton
VX5700



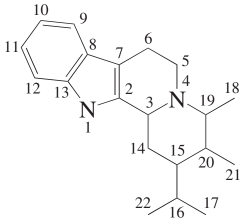
Kopsane skeleton
VX5560



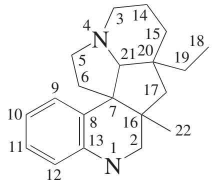
Koumine skeleton
VX5150



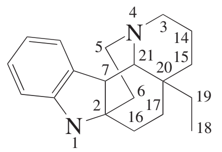
Macroline skeleton
VX4900



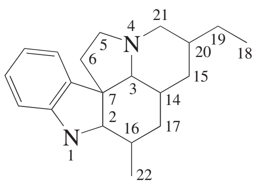
Malindan skeleton
VX4920



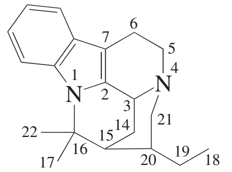
Melodinus skeleton
VX5580



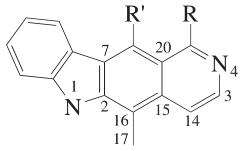
Melonine skeleton
VX5460



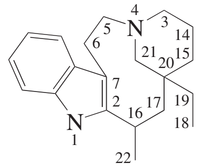
Pandoline skeleton
VX5800



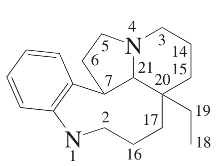
Pleiocarpaman skeleton
VX5220



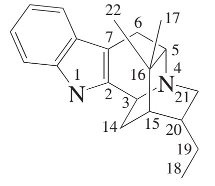
Pyridocarbazole skeleton
VX5840



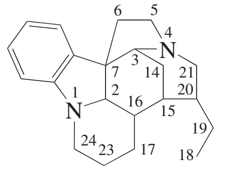
Quebrachamine skeleton
VX5500



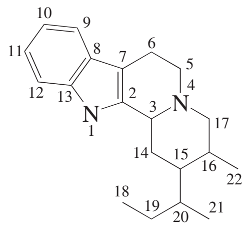
Rhazinilam skeleton
VX5450



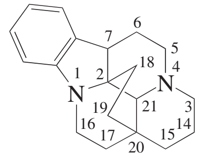
Sarpagine skeleton
VX5100



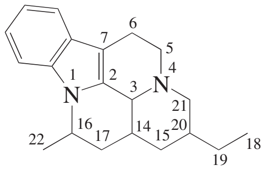
Strychnidine skeleton
VX5280



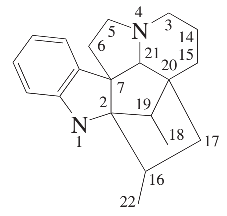
Vallesiachotaman skeleton
VX4960



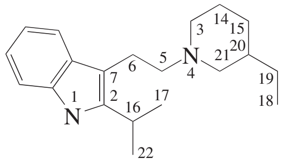
Schizozygine skeleton
VX5930



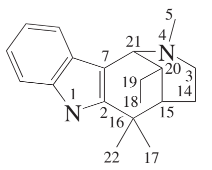
Tacaman skeleton
VX5920



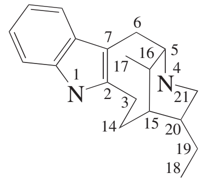
Vindolinine skeleton
VX5550



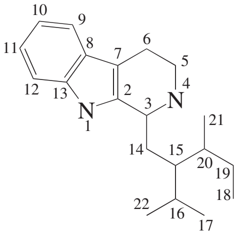
Secodine skeleton
VX5360



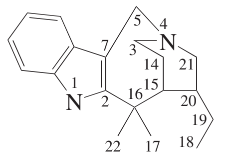
Ulean skeleton
VX5860



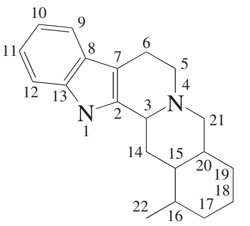
Vobasine skeleton
VX5140



Strictosidine skeleton
VX4640



Vallesaman skeleton
VX5880



Yohimbinoid skeleton
VX5040

In the main types of indole alkaloids having the secologanin subunit in unrearranged form, stereoisomerism at positions 3, 19, and 20 is common, but *C*-15 is invariant based on the corresponding carbon in secologanin. *C*-22 is frequently absent (for example, in all known actual alkaloids of the Pleiocarpamine group VX5220), but is shown in the skeletons.

Some indole alkaloids in various groups are found as variants resulting from indole to indoxole or pseudoindoxyl rearrangement. These are often treated as a separate category, oxindole alkaloids, but here they have been listed under the corresponding parent indole structure type (change from the first edition), as new types continue to be found. For example, **Rhynchophylline**, based on the corynoxan skeleton, is here categorised as a corynanthe alkaloid, VX4800. Another type of rearrangement found in some of the groups (Camptothecins, Cinchona alkaloids) is conversion of the indole to a quinoline nucleus. This means that the resulting structures do not strictly speaking contain an indole nucleus. However, they are considered to be indole alkaloids on biogenetic grounds.

Indole alkaloids are most common in the Apocynaceae, Loganiaceae and Rubiaceae, and are also found in the Alangiaceae, Icacinaceae, Nyssaceae, and possibly other families.

The Chemistry of Heterocyclic Compounds: Indoles-The Monoterpenoid Indole Alkaloids, (ed, Saxton, J.E.), Wiley, 1983, **25**, part 4; supplement, 1994 (*rev, bibl*)
Saxton, J.E., *Nat. Prod. Rep.*, 1997, **14**, 559–590 and earlier (*revs*)
Verpoorte, R. *et al., Alkaloids*, 1997, **49**, 221–299 (*rev*)
Leonard, J., *Nat. Prod. Rep.*, 1999, **16**, 301–318 (*rev*)
O'Connor, S.E. *et al., Nat. Prod. Rep.*, 2006, **23**, 532–537 (*rev, biosynth*)
Szabó, L.F., *J. Phys. Org. Chem.*, 2006, 19, 579–591 (*rev, classification*)
Szabó, L.F., *Molecules*, 2008, 13, 1875–1896 (*rev, classification*)

Strictosidine alkaloids (VX4640)

This category covers alkaloids related to the biogenetic parent alkaloid **Strictosidine** without further carbon-skeleton modification.

Camptothecin alkaloids (VX4700)

These alkaloids, which contain the quinoline ring system, are probably derived from Strictosidine via an intermediate related, possibly, to **Rubescine**. In this case, conversion of the indole group into the quinoline ring involves ring enlargement of ring B at the expense of ring C; otherwise the changes in the formation of **Camptothecin** from Strictosidine are straightforward.

Soepenberg, O. *et al., Alkaloids*, 2003, **60**, 1–50 (*rev*, *biochem*)

Corynanthean alkaloids (VX4800)

This large group, formed by simple cyclisation of the precursor, is exemplified by **Geissoschizine** and **Sitsirikine**.

In corynanthe alkaloids and other groups closely related to them (e.g. yohimbanes, below), stereoisomeric variation is common except at *C*-15, which is invariably 15α*H*-.

Szántay, C. *et al., Alkaloids,* 1986, **27**, 131–269 (*rev*)

Secologanin-derived sesquimer alkaloids (VX4820)

These are derived from two biogenic amine subunits and one monoterpenoid subunit (normal sesquimers), or one biogenic amine subunit and two secologanin units (reversed sesquimers). The greatest number are formed by condensation of a (usually) Corynanthe portion with an additional tryptamine or canthine subunit, as in the **Ochrolifuanines** and **Usambarensines.** The dictionary entries carry the code numbers for the constituent fragments also.

Brown, R.T., *The Chemistry of Heterocyclic Compounds: Indoles-The Monoterpenoid Indole Alkaloids*, (ed. Saxton, J.E.), Wiley, 1983, **25**, part 4, 63–146 (*rev*)
Kam, T.-S. *et al., Alkaloids,* 2006, **63**, 181–337 (*rev*)

Akageran and related alkaloids (VX4840)

This relatively small group of alkaloids typified by **Akagerine** appears to be formed by bond-breaking of a corynanthe precursor followed by formation of a 7-membered ring. Included here are a small number related to **Adifoline**.

Ajmalicine-like alkaloids (VX4860)

These are based on a 17,19-secoyohimban skeleton which is invariably present as an ether (oxayohimban). **Ajmalicine** was formerly considered a key intermediate in indole alkaloid biosynthesis, but this has been disproved.

Lewis, S.E., *Tetrahedron*, 2006, **62**, 8655–8681 (*rev*)

Macroline alkaloids (VX4900)

This group is related to the Akuammilines (VX5200 below) by scission of the *C*-21 to *N*-4 bond. The macroline skeleton mostly occurs in bisindole alkaloids; Macroline itself has not yet been found as a free alkaloid and only a small number of monomeric analogues are known.

MALINDAN ALKALOIDS; CADAMBAN ALKALOIDS; VALLESIACHOTAMAN ALKALOIDS (VX4920, VX4940, VX4960)

See chart. These are small groups, e.g. **Malindine; Cadambine, Vallesiachotamine**, some alkaloids having an elaborate additional pyridine ring.

GELSEMIUM ALKALOIDS (VX5000)

These alkaloids contain an oxindole function and a cage-like, hydroaromatic residue which can be imagined, in a formal sense, to arise from an intermediate related to anhydrovobasinediol by formation of a 6,20 bond and rearrangement to an oxindole. The major alkaloids in this group are related to **Gelsemine**; however, a smaller group, characterised by **Gelsedine**, lack the 6,20 bond, and have also lost *C*-21.

Takayama, H. *et al., Alkaloids,* 1997, **49**, 1–78 (*rev*)

YOHIMBINOID ALKALOIDS (VX5040)

The Yohimbinoid alkaloids contain a carbocyclic ring E arising through *C*-17 to *C*-18 bond formation in a corynantheine precursor. As in the corynantheine and ajmalicine groups, stereoisomerism at all chiral centres, except *C*-15, is known. Structural variations include the presence of methoxy-groups in the aromatic ring, hydroxy- or acyloxy- groups at *C*-18, as in **Reserpine**, and various degrees of unsaturation in rings C-E, as in **Alstoniline**.

Brown, R.T., *The Chemistry of Heterocyclic Compounds: Indoles-The Monoterpenoid Indole Alkaloids*, (ed. Saxton, J.E.), Wiley, 1983, **25**, part4, 147–199 (*rev*)
Szántay, C. *et al., Alkaloids*, 1986, 27, 131–269 (*rev*)
Baxter, E.W. *et al., Alkaloids Chem. Biol. Perspect.*, 1990, **8**, 197–319 (*rev, synth*)

SARPAGINE ALKALOIDS (VX5100)

The Sarpagine (Akuammidine) group, based on the sarpagan nucleus, arises from bond formation between *C*-16 and *C*-5 of the corynantheine precursor and consists of simple **Akuammidine** derivatives and oxindoles obtained following the migration of *C*-3 from *C*-2 to *C*-7, e.g. **Gardneramine.** The closely related Vobasine (VX5140) and Ervatamia (VX5180) groups are now listed separately.

Joule, J.A., *The Chemistry of Heterocyclic Compounds: Indoles-The Monoterpenoid Indole Alkaloids*, (ed. Saxton, J.E.), Wiley, 1983, **25**, part 4, 201–264 (*rev*)
Hamaker, L.K. *et al, Alkaloids Chem. Biol. Perspect.*, 1994, **9**, 23–84 (*rev, synth*)
Lounasmaa, M. *et al., Alkaloids*, 1999, **52**, 103–195 (*rev*)
Lewis, S.E., *Tetrahedron*, 2006, **62**, 8655–8681 (*rev*)

AJMALINE ALKALOIDS (VX5120)

The ajmaline group contains both 5,16 and 7,17 bonds. **Ajmaline** itself is the best known example. Almost all the bases in this group contain the same skeleton, but **Perakine** and its congeners afford a rare structural variation in which the 21,*N* bond has been replaced by a 19,*N* bond.

Lewis, S.E., *Tetrahedron*, 2006, **62**, 8655–8681 (*rev*)
Lounasmaa, M. *et al., Alkaloids*, 2001, **55**, 1–87 (*rev*)

VOBASINE ALKALOIDS (VX5140)

These are related to the sarpagine group by C-3 to *N*-4 bond scission.

KOUMINE ALKALOIDS (VX5150)

These are 7,20-cyclovobasine alkaloids.

ERVATAMIA ALKALOIDS (VX5180)

These alkaloids (e.g. **Ervatamine**, **Methuenine**) can be successfully produced *in vitro* from vobasine-type alkaloids (VX5140) and this has also been achieved by enzymic preparations. The process involves 5,6- bond cleavage and 6,16- bond formation.

Thai, C. *et al.*, *J.A.C.S.*, 1981, **103**, 4956–4957 (*biosynth*)

AKUAMMILINE ALKALOIDS (VX5200)

The ring system in this group is formed from a precursor of the corynantheine type by bond formation between *C*-16 and *C*-7. In addition to close relatives of **Akuammiline**, variations in this subgroup include alkaloids derived by *C*-3 to *N*-4 bond fission and *C*-2 to *N*-4 bonding, e.g. **Echitamine,** and alkaloids in which the *N*-4 to *C*-5 bond in the Akuammiline skeleton has been severed, e.g. **Aspidodasycarpine**. **Nareline** is a unique alkaloid with an additional bond between *C*-21 and *C*-6.

Lewis, S.E., *Tetrahedron*, 2006, **62**, 8655–8681 (*rev*)

PLEIOCARPAMAN ALKALOIDS (VX5220)

In this group, a corynantheine precursor has cyclised via *C*-16 on to *N*-1, as in **Pleiocarpamine**.

Gilbert, B., *Alkaloids*, 1968, **11**, 205–306 (*rev*)

CINCHONA ALKALOIDS (VX5240)

This important and well-known group, which includes the valuable antimalarial quinine, consists of two subgroups: the **Cinchonamine** group, derived from a corynantheine-type precursor by fission of the *N*-4 to *C*-5 bond plus attachment of *N*-4 to *C*-17, and the **Quinine** group, which contain a quinoline ring system generated from a precursor of the cinchonamine type by 2,7-bond fission followed by bonding of *N*-1 to *C*-5. **Corialstonine** represents an abeo-variant.

Grethe, G. *et al., The Chemistry of Heterocyclic Compounds: Indoles-The Monoterpenoid Indole Alkaloids*, (ed. Saxton, J.E.), Wiley, 1983, **25**, part 4, 729–752 (*rev*)
Hoffmann, H.M.R. *et al., Eur. J. Org. Chem.*, 2004, 4293–4312 (*rev*)

AKUAMMICINE (CURAN) ALKALOIDS (VX5260)

The biogenesis of these alkaloids presumably involves migration of *C*-3 in a corynanthe precursor from *C*-2 to *C*-7, followed by formation of the 2,16-bond. An early alkaloid in the group is therefore **Preakuammicine,** which loses formaldehyde to give **Akuammicine**. Included in this group is **Stemmadenine**, a 3,7-secoalkaloid which appears to be the intermediate on the pathway to the Ulean group below (VX5860).

STRYCHNIDINE ALKALOIDS (VX5280)

Formation of the skeleton of these typical *Strychnos* alkaloids involves the addition of two carbon atoms to a curan precursor, presumably, from an acetate unit

Husson, H,-P., *The Chemistry of Heterocyclic Compounds: Indoles-The Monoterpenoid Indole Alkaloids*, (ed. Saxton J.E.), Wiley, 1983, **25**, part 4, 293–330 (*rev*)
Bosch, J. *et al., Alkaloids*, 1996, **48**, 75–189 (*rev*)
Ohshima, T., *Chem. Pharm. Bull.*, 2004, **52**, 1031–1052 (*rev, synth*)
Shibasaki, M. *et al., Alkaloids*, 2007, **64**, 103–138 (*rev, synth*)

CONDYLOCARPAN ALKALOIDS (VX5320)

These alkaloids contain a ring system similar to that of the curan group, but are formed by cyclisation of *C*-21 on to *C*-7 in a Corynanthe precursor, rather than the formation of a 3,7 bond; **Condylocarpine** is representative. Note that loss of the ethanamine carbons 5 and 6 gives the ring system of uleans (VX5860 below), which thus suggests an alternative biogenetic route to the one given below. Extensive modification of this skeleton appears to have occurred in the formation of **Goniomine**, which can be postulated to be formed by ring-opening and epoxidation of an indolenine related to Condylocarpine followed by *N*-1 to *C*-19 bonding.

Lounasmaa, M., *Prog. Chem. Org. Nat. Prod.*, 1986, **50**, 27–56 (*rev*)

SECODINE ALKALOIDS (VX5360, VX4740)

This group of tricyclic alkaloids is formed by ring-opening of a precursor of the Preakuammicine type. The alkaloids occur in various stages of reduction, and in monomeric and dimeric forms. **Andranginine**, the product of an unusual cyclisation of a dehydrosecodine, may also be included here.

Hájiček, J., *Collect. Czech Chem. Commun.*, 2004, **69**, 1681–1767 (*rev*, *synth*)

ASPIDOSPERMA ALKALOIDS (VX5400)

The skeleton of the aspidospermidine alkaloids is formed by cyclisation of a dehydrosecodine, itself obtained from a precursor related to Preakuammicine. The alkaloids in this group are based on several structural variants. A methoxycarbonyl group at *C*-16 may be present (**Tabersonine**) or absent (**Aspidospermine)**; in each case, *C*-18/*C*-19 may be an ethyl group, or may be functionalised, e.g. into a lactone system. **Obscurinervidine** contains a dihydro-1,4-oxazine ring between *N*-1 and *C*-12.

Saxton, J.E., *The Chemistry of Heterocyclic Compounds: Indoles-The Monoterpenoid Indole Alkaloids*, (ed. Saxton, J.E.), Wiley, 1983, **25**, part 4, 331–437 (*rev*)
Overman, L.E. *et al., Alkaloids Chem. Biol. Perspect.*, 1985, **3**, 275–307 (*rev*)
Cordell, G.A., *Alkaloids*, 1997, **50**, 327–384 (*rev*)
Saxton, J.E., *Alkaloids*, 1998, **51**, 1–197 (*rev*)
Hájiček, J., *Collect. Czech Chem. Commun.*, 2004, **69**, 1681–1767 (*rev, synth*)

RHAZINILAM ALKALOIDS (VX5450)

These are alkaloidal artifacts related to the aspidosperma group by *C*2-*C*7 fission, the indole functionality thus being lost.

Hájiček, J., *Collect. Czech Chem. Commun.*, 2007, **72**, 821–898 (*rev*, *synth*)

MELONINE ALKALOIDS (VX5460)

This small group has undergone a (6 →2) abeo shift from an Aspidosperma-like precursor.

QUEBRACHAMINE ALKALOIDS (VX5500)

Quebrachamine alkaloids are derived from the Aspidosperma group (type III skeleton) by fission of the 7,21-bond. They may have lost the *C*-16 methoxycarbonyl group (e.g. **Quebrachamine**) or it may have been retained, as in **Vincadine**.

Hájiček, J., *Collect. Czech Chem. Commun.*, 2004, **69**, 1681–1767; 2007, **72**, 821–898 (*rev*, *synth*)

ASPIDOFRACTINE ALKALOIDS (VX5540)

These are related to the Aspidosperma group by formation of a *C*-2 to *C*-18 bond.

Hájiček, J., *Collect. Czech Chem. Commun.*, 2007, **72**, 821–898 (*rev*, *synth*)

VINDOLININE ALKALOIDS (VX5550)

These are related to the Aspidosperma group by formation of a *C*-2 to *C*-19 bond.

KOPSANE ALKALOIDS (VX5560)

The skeleton of the kopsane group of alkaloids is simply formed by attachment of *C*-22 (the methoxycarbonyl carbon) of Venalstonine to *C*-6, as in **Kopsine**. Skeletal variations include the alternative acyloin structure, as in **Fruticosine**, in which *C*-22 is attached to *C*-17.

Hájiček, J., *Collect. Czech Chem. Commun.*, 2007, **72**, 821–898 (*rev*, *synth*)
Kam, T. S. *et al., Alkaloids,* 2008, **66**, 1–111 *(rev)*

MELODINUS ALKALOIDS (VX5580)

These have been isolated only from *Melodinus* and *Kopsia* spp. (e.g. **Meloscine**, **Scandine**). They are plausibly biosynthesised from alkaloids of the Tabersonine type (VX5400). There are two known dimer alkaloids.

Hugel, G. *et al., J.O.C.*, 1986, **51**, 1594–1595 (*biosynth*)

IBOGA ALKALOIDS (VX5700)

A further mode of cyclisation of a secodine-type precursor involves formation of a 16,21 bond, which gives rise to the bridged ring system (type II indole alkaloid) found in **Ibogamine**, **Catharanthine**, and numerous related alkaloids. They are often components of heterodimer indole alkaloids.

This group of alkaloids exists in both enantiomeric series which may be defined by the chirality of *C*-14. The best-known example of the 14*S* series is Catharanthine. Most other alkaloids of this group belong to the 14*R* series. Many alkaloids retain the methoxycarbonyl group, whereas others (e.g. Ibogamine) have lost it. Other variations include oxidation at *C*-7 to give the related hydroxyindolenines, e.g. **Iboxygaine hydroxyindolenine**; oxidation followed by rearrangement to the related indoxyl, e.g. **Desmethoxyiboluteine**, oxidative rearrangement to the corresponding oxindole, as in **Tabernoxidine**; and oxidation at *C*-19, *C*-3, *C* -5, or *C*-6 with, occasionally, ether formation between oxidised positions.

Also **16-Hydroxyalloibogamine**, the only alkaloid having the analogous but isomeric bridged ring system (type III skeleton) is also ranked into this class of alkaloids.

Cordell, G.A., *The Chemistry of Heterocyclic Compounds: Indoles-The Monoterpenoid Indole Alkaloids*, (ed. Saxton, J.E.), Wiley, 1983, **25**, part 4, 467–537 (*rev*)
Popik, P. *et al., Alkaloids*, 1998, **52**, 197–231 (*rev, pharmacol*)
Sundberg, R.J. *et al., Alkaloids*, 2002, **59**, 281–366 (*rev*)
Hájiček, J., *Collect. Czech Chem. Commun.*, 2004, **69**, 1681–1767 (*rev, synth*)

PANDOLINE ALKALOIDS (VX5800)

The Pandoline (pseudoaspidospermidine) (type II indole alkaloid) nucleus can be imagined to be formed by cyclisation of a secodine derivative isomeric with that postulated as a precursor for Aspidospermidine. **Ibophyllidine** represents an obvious ring contraction, **Iboxyphylline** a ring extension.

CLEAVAMINE ALKALOIDS (VX5820)

The small **Cleavamine** group is more often encountered as degradation products of other alkaloids; these may arise by fission of the 3,7-bond. Alternatively, and perhaps more likely, this ring system can be generated by fission of the 16,21-bond in an Iboga skeleton (see below).

Hájiček, J., *Collect. Czech Chem. Commun.*, 2004, **69**, 1681–1767; 2007, **72**, 821–898 (*rev*, *synth*)

PYRIDOCARBAZOLE ALKALOIDS (VX5840)

This small and pharmacologically important group is based on the 6*H*-pyrido[4,3-*b*]carbazole ring system, and is exemplified by **Ellipticine** and **Olivacine**. Although these aromatic bases may superficially seem to be unrelated to the mainstream indole monoterpenoid alkaloids a possible biogenesis from Stemmadenine can be postulated. However, the details of the biosynthesis do not appear to have been investigated experimentally since the 1970s, when only low incorporation of tryptophan was found.

There are two subtypes in that Ellipticine is derived biogenetically from the Ajmalicine type (VX4860) and Olivacine from the Malindan type (VX4920). Because of this biogenetic diversity and their separation structurally from the mainstream indole alkaloids, systematic (CAS) numbering is now usually employed in the literature for the ellipticine nucleus.

Gribble, G.W. *et al.*, *Heterocycles*, 1985, **23**, 1277–1315 (*rev*, *synth*)
Kansai, V.K. *et al.*, *Tetrahedron*, 1986, **42**, 2389–2408 (*rev*)
Alvarez, M. *et al., Alkaloids*, 2001, **57**, 235–272 (*rev*)

ULEAN AND VALLESAMAN ALKALOIDS (VX5860, VX5880)

These alkaloids may well arise, like the Ellipticine group, from an oxidative fission of a Stemmadenine-like intermediate. The genesis of the three types, e.g. **Vallesamine**, **Uleine**, and **Apparicine** can thus readily be explained.

Joule, J.A., *The Chemistry of Heterocyclic Compounds: Indoles-The Monoterpenoid Indole Alkaloids*, (ed. Saxton, J.E.), Wiley, 1983, **25**, part 4, 265–292 (*rev*)
Alvarez, M. *et al., Alkaloids*, 2001, **57**, 235–271 (*rev*)

EBURNA AND SCHIZOZYGINE ALKALOIDS (VX5900; VX5930)

The skeleton of the Eburna alkaloids is generated by rearrangement of the aspidospermidine ring system, involving migration of *C*-21 from *C*-7 to *C*-2, fission of the 2,16-bond, and attachment of *C*-16 to *N*-1. This rearrangement has been very successfully imitated *in vitro*. **Vincamine** and its derivatives retain the methoxycarbonyl group; **Eburnamine** and **Eburnamenine** have lost it. There are some alkaloids in which *C*-18 or *C*-19 is oxidised, e.g. **Cuanzine**.

The **Schizozygine** group (VX5930) contain an additional bond between *C*-2 and *C*-18. Included are **Andrangine** and **Vallesamidine**, which can be considered as secoschizozygines or as Eburna alkaloids in which *C*-21 has simply migrated to *C*-2.

Saxton, J.E., *The Chemistry of Heterocyclic Compounds: Indoles-The Monoterpenoid Indole Alkaloids*, (ed. Saxton, J.E.), Wiley, 1983, **25**, part 4, 439–465 (*rev*)
Lounasmaa, M. *et al., Alkaloids*, 1992, **42**, 1–116 (*rev*)

TACAMAN ALKALOIDS (VX5920)

A small group is apparently obtained by processes analogous to the formation of the Eburna group, but from a precursor to a pseudoaspidospermidine (type II skeleton) derivative, by the formation of new bonds at *C*-2→*C*-3 and *C*-14→*C*-17. Again, *C*-22 may be present (**Tacamine**) or absent (**Tacamonine**).

Danieli, B. *et al., Alkaloids*, 1986, 27, 95–103 (*rev*)

CHIPPIINE ALKALOIDS (VX5940)

These represent a numerically limited group. Their structures can be derived from an Iboga-type precursor by cleavage of the *C*-3 to *N*-4 bond and formation of an *N*-1 to *C*-3 bond.

BISINDOLE ALKALOIDS (VX5980)

This large group of complex alkaloids consists of a wide variety of structures, depending on the identity of the monomeric alkaloid components. The individual alkaloids are normally coded in addition with the Type of Compound codes relevant to the component halves of the molecule. (e.g. **Conodurine** = a Vobasine (VX5140)-Iboga (VX5700) dimer). The most practically important indole alkaloid dimers are those of the Cleavamine-Aspidosperma group. **Vinblastine** and **Vincristine** are the best known examples.

Whilst in these dimers and many others the monomeric units are linked by single covalent bonds, in others the assembly is more complex. The **Vobtusine** group, for example, is composed of two aspidospermidine-type units linked by a spirocyclic system involving *C*-14 (two bonds) of one unit with *C*-22′ of another unit, together with an additional carbon atom attached to *N*-1′. A small group contains three inter-unit bonds as in **Ervafoline**.

Other types of dimeric alkaloids from *Strychnos* Spp. form the major constituents of calabash curare. These are composed of two units linked via *N*-1 and *C*-17′, and *N* -1′ and *C*-17; ***C*-Toxiferine** is representative. In some alkaloids additional bonds are present; for example, ***C*-Curarine** has an ether bridge between *C*-16 and *C*-16′, and ***C*-Calebassine** has an additional carbon-carbon bond between *C*-17 and *C*-17′.

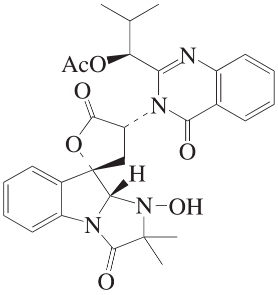
Cordell, G.A, *Alkaloids,* 1981, **20**, 3-295; 1983, **25,** 539–728 (*revs*)
Hájiček, J., *Collect. Czech Chem. Commun*., 2004, **69**, 1681–1767; 2007, **72**, 821–898 (*rev*, *synth*)
Kam, T.-S. *et al., Alkaloids*, 2006, **63**, 181–337 (*rev*)

ISOINDOLES (VX6000)

This is a heterogeneous group including terpenoids which are also coded as such. Small isoindoles include microbial products, e.g. **Cichorine.**

TRYPTOQUIVALINES (VX6030)

The **Tryptoquivalines**, which are toxic metabolites from *Aspergillus clavatus*, are derived from anthranilic acid and tryptophan precursors, and half of the molecule is related to the Quinazoline alkaloids above (VX1600). The reviews of quinazoline alkaloids cited there normally cover the tryptoquivalines.



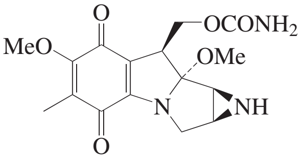
Tryptoquivaline A

There has been some uncertainty concerning their absolute configurations. It seems now established that they all have the (2*S*,3*S*,12*R*)- stereochemistry, but in the case of a few of the tryptoquivalines corrected stereochemistries have not been published.

The group also includes some more recently isolated analogues such as the **Fumiquinazolines.**

MITOMYCINS (VX6050)

This is a small group of purple microbial pigments (their typical representative is **Mitomycin A**) showing antitumour properties. They are usually quinones containing an aziridinyl function. They are biosynthesised from 3-amino-5-hydroxybenzoic acid, the aziridine nitrogen coming from glucosamine. The **Albomitomycins**, rearrangement products of mitomycins, contain a diazatricyclic ring system unique among natural products.

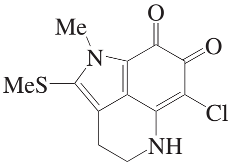


Mitomycin A

Remers, W.A. *et Alkaloids Chem. Biol. Perspect.*, 1987, **5**, 1–74 (*rev*)

PYRROLO[4,3,2-*DE*]QUINOLINE ALKALOIDS (VX6070)

This skeleton is characteristic of and almost exclusive to marine (sponge) alkaloids. Major subgroups include the simple **Batzellines**, **Makaluvamines** and **Damirones**, and those in which the pyrroloquinoline nucleus forms part of a larger skeleton such as in the **Discorhabdins** and the closely related **Epinardines**. They are thought to be biosynthesised from tyrosine via **3,5-Dibromoverongiaquinol**.



Batzelline A

Ding, Q. *et al.*, *Curr. Med. Chem.*, 1999, **6**, 1–27 (*rev*)

MISCELLANEOUS INDOLE ALKALOIDS (VX6100)

Under this heading are listed indole alkaloids for which a classification remains premature, either because they currently belong to a very limited subtype, and/or because there has been no work on their biosynthesis. Many of them probably represent minor branches on the biosynthetic pathways to the larger groups; for example the **Rhopaladins** are probably biosynthetically close to the indolo[2,3-α]carbazole alkaloids (VX4350), but this is not yet established experimentally. **Granulatimide** may represent a lower benzologue of these alkaloids incorporating a histamine residue in place of one tryptamine. Plant alkaloids representing variations in skeleton of which only one or two examples are known include **Pandine**, **Iboxyphylline** and **Ibophyllidine** (all skeletal variations apparently related to the Pandoline type). Others are degraded indole alkaloids of unknown parental type.

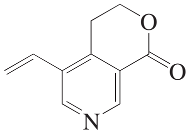
Somei, M. *et al.*, *Nat. Prod. Rep.*, 2004, **21**, 278–311 (*rev*)
Kawasaki, T. *et al.*, *Nat. Prod. Rep.*, 2005, **22**, 761–793 (*rev*)

TERPENOID ALKALOIDS (VX6240–VX6500)

Further information on terpenoid structures and biosynthesis generally can be found in the *Dictionary of Natural Products.*

Monoterpenoid alkaloids (VX6240)

This is a diverse group. The carbon skeleton is mostly C_{10}, but in many alkaloids it is C_9 and in some it is C_{11}. There are two major groups; those derived from iridodial-like precursors, e.g. **α-Skytanthine**, and those derived from Secologanin, typified by **Gentianine**, **Bakankoside**, and **Gentioflavine**. However, this heading also covers a variety of miscellaneous amines and amides based on small terpenoid skeletons, e.g. **Alfileramine** (menthane-type) and **Fontaineine** (simple acyclic monoterpenoid).



Gentianine

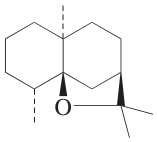
Cordell, G.A., *Alkaloids*, 1998, **52**, 260–327 (*rev*)

Sesquiterpene alkaloids (VX6300)

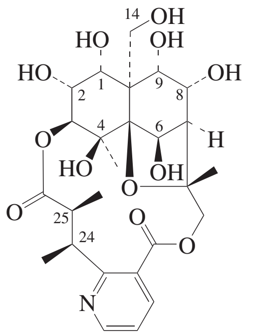
A variety of sesquiterpene alkaloids have been isolated from plant (e.g. **Guaipyridine**; **Muscicapines**) and marine sources and are nearly all relatively simple amine or amide derivatives of well-known sesquiterpenoid (or meroterpenoid) skeletons. They may be acyclic (e.g. **Axinyssimides**), monocyclic (**Smenospongine**) or bicyclic (**Nakijiquinones**).

Macrocyclic sesquiterpene alkaloids (VX6320)

This group of plant alkaloids contains the ring system of dihydroagarofuran, a sesquiterpene of the eudesmane group, esterified with nicotinic acid, or with any of several dicarboxylic acids. Most of the alkaloids, which occur in *Euonymus* and *Maytenus* species among others, contain a medium ring dilactone involving one of the dicarboxylic acids; **Evonine** is typical. Some alkaloids with two dilactone medium rings have also been isolated.



Dihydroagarofuran

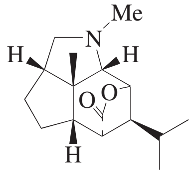


Per(deacyl)euojaponin

In the dictionary entries, series of these alkaloids which are esters of the same basic skeleton are usually shown as derivatives of the parent polyol, such as **Per(deacyl)euojaponin** (parent alkaloidal polyol of the **Euojaponins** and of various other alkaloids, e.g. **Cathedulins**). The names chosen for these parent structures (often uncharacterised as such) in the Dictionary are chemically reasonable, but may not be found elsewhere in the literature.

Dendrobium alkaloids (VX6340)

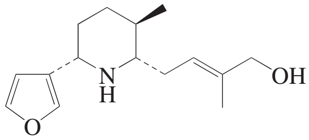
These alkaloids fall biogenetically into two quite distinct groups; a group of sesquiterpene alkaloids typified by **Dendrobine**, from *Dendrobium nobile*, with variants involving oxygenation at *C*-2 or *C*-6, and fission of the nitrogen to *C*-2 bond, and a group of indolizidine bases exemplified by **Crepidamine** from *Dendrobium crepidatum*. These are probably not terpenoid in origin, and may be derived from shikimic acid, acetate, and ornithine.



Dendrobine

NUPHAR ALKALOIDS (VX6360)

The *Nuphar* (water-lily) alkaloids contain a normal sesquiterpene carbon skeleton, and can be divided into two main sub-groups: furylpiperidines, e.g. **Nuphamine**; and furylquinolizidines, e.g. **Deoxynupharidine**. The latter group includes a number of sulfur-containing dimers such as **Neothiobinupharidine**, plus a few miscellaneous bases. A number of these alkaloids have also been isolated from the scent glands of beavers, *Castor* spp., acquired presumably by a dietary route.

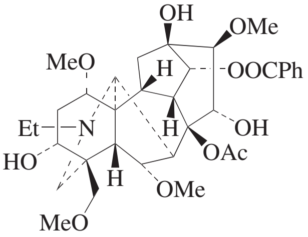


Nuphamine

Wróbel, J.T., *Alkaloids*, 1977, **16**, 181–214 (*rev*)
Cybulski, J. *et al., Alkaloids*, 1989, **35**, 215–257 (*rev*)
Michael, J.P., *Nat. Prod. Rep.*, 2004, **21**, 625–649; 2005, **22**, 603–626; 2008, **25**, 139–165 (*revs*)

C_{19} AND C_{20} DITERPENOID ALKALOIDS AND 4-NOR ANALOGUES (VX6400, VX6420)

These alkaloids are very numerous and include some highly toxic bases with strong physiological properties, such as **Aconitine**. Although they are obviously diterpenoid in origin, few biogenetic studies have been reported, apart from relatively early reports of the incorporation of acetate and mevalonate into **Browniine** and **Lycoctonine**, and of mevalonate and glycine into **Delcosine**. A recent hypothesis suggests their formation directly from the complete diterpenoids by a process involving Mannich reactions.



Aconitine

The first group (VX6400) is based on the C_{19} aconitane ring system, characteristic of the Ranunculaceae. Alkaloids of this group are fairly homogeneous structurally and differ only in the pattern of substitution by hydroxy, methoxy, acetyloxy, benzoyloxy and, frequently, anthranilate-based groups (e.g. **Delsemines**), although recently other structural variations such as unsaturation and epoxidation have been found.

The simpler alkaloids are collected in the Dictionary under the parent aconitane skeleton. Note that in the CAS parent aconitane, *C*-18 is missing, and following CAS nomenclature, the parent skeleton is 4-methylaconitane. The extra carbon atom is numbered *C*-18.

A few alkaloids belong to the heteratisane group, formed from the aconitane framework by oxidative fission of the 13,14-bond.

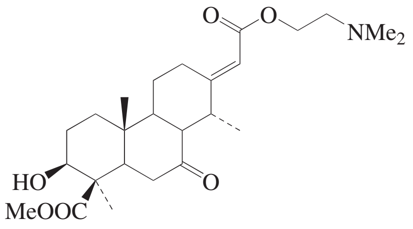
The second major group are the C_{20} alkaloids (VX6420), based on atidane and more widely distributed among dicot families. Few alkaloids, as it happens, are based on the parent ring system, since many skeletal variations are known. These include the hetisans (e.g. **Davisine**), in which additional rings are introduced into the atidane ring system by formation of 14,20 and *N*,6 bonds. The unmodified hetisans are presented in the Dictionary under the systematic hetisan name. There is a small group of atidane 7,20 cyclic ethers (**Ajaconine**) and various other modifications involving ring fission, contraction, migration etc. of the hetisan skeleton (**Denudatine**, **Delnudine**, **Cardionidine**, etc.)

Another major modification leads to the veatchine skeleton, as in **Cuauchichicine**. There are also 7,20-Cycloveatchine bases, e.g. **Lucidusculine**, 14,20-Cycloveatchine bases, e.g. **Anopterine** and miscellaneous bases.

Pelletier, S.W. *et al., Alkaloids*, 1979, **17**, 2–104; 1981, **18**, 100–216 (*revs*)
Benn, M.H. *et al., Alkaloids Chem. Biol. Perspect.,* 1983, **1**, 153–210 (*toxicity*, *pharmacology*)
Amiya, T. *et al.*, *Alkaloids*, 1988, **34**, 95–179 *(rev)*
Joshi, B.S. *et al.*, *Alkaloids Chem. Biol. Perspect.,* 1999, **13**, 289–370; 2001, **15**, 1–414 (*revs*, *pmr*, *cmr*)
Wang, F. P. *et al.*, *Alkaloids*, 2002, **59**, 1–280 *(rev)*

ERYTHROPHLEUM ALKALOIDS (VX6460)

The alkaloids of *Erythrophleum* spp. (Fabaceae) are based on the diterpene skeleton related to Cassaic acid. The oxidation pattern is relatively simple, involving only *C*-3, *C*-6, *C*-7 and *C*-19. In most alkaloids, *C*-19 is at the carboxylic acid oxidation level. All the alkaloids are esters or amides of a *C*-16 carboxylic acid with *N*,*N*-dimethylethanolamine or *N*-methylethanolamine. **Erythrophlamine** is a typical example. There have been some confusing structure revisions in this series; they have been little studied recently.

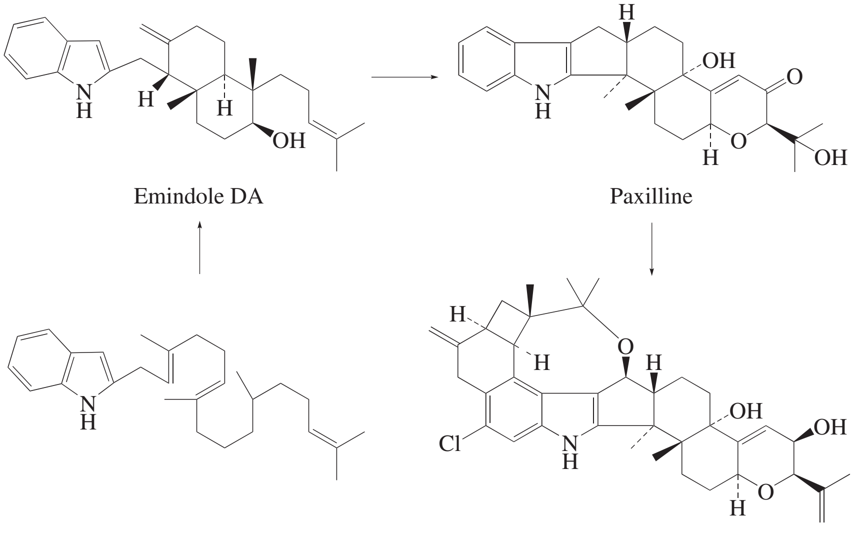


Erythrophlamine

Morin, R.B., *Alkaloids*, 1967, **10**, 287–303 (*rev*)

PENITREMS (VX6470)

This heading covers indoloterpenoid metabolites from microorganisms including the **Penitrems**, **Emindoles**, **Nodulisporic acids** and others. They are mostly toxic, many with tremorigenic activity. The intermediary of **Emindole DA** and **Paxilline** in their biosynthesis from geranylindole has been recently demonstrated. **Shearinine I** is an interesting ring-cleaved compound which has lost the indolo functionality.



Emindole DA

Paxilline

Penitrem C

Steyn, P.S., *Prog. Chem. Org. Nat. Prod.*,1985, **48**,1–80 (*rev*)
Sings, H. *et al.*, *Alkaloids,* 2003, **60**, 51–163 (*rev*)
Fueki, S. *et al.*, *Org. Lett.*, 2004, **6**, 2697–2700 (*biosynth*)

MISCELLANEOUS DITERPENOID ALKALOIDS (VX6480)

This category includes diterpenes linked by an ester function to a non-terpenoid nitrogen-containing unit. Examples are **Ryanodine**, **Concavine** and the **Decaturins**. The **Agelasines**, **Agelasimines** and related alkaloids are a series of guanidinoid- or purinoid- substituted simple acyclic, mono- or bi-cyclic terpenoids, and there are one or two simple amino-substituted cembranoids.

Appendino, G. *et al., Alkaloids Chem. Biol. Perspect.*, 1996, **11**, 237–268 (*rev, Taxus alkaloids*)

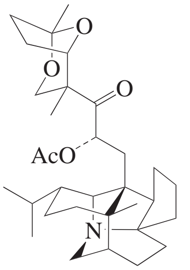
SESTERTERPENE ALKALOIDS (VX6490)

A few nitrogen-containing sesterterpenoids are present in marine organisms, however, the number so far characterised is relatively low in comparison with the number of nitrogen-free tetracyclic sesterterpenes, which are common in marine organisms. The **Spongidines** and the **Molliorins**, in which a ring-E pyridine or pyrrole ring, respectively, is fused to one of the common tetracyclic skeletons, are the main types. There are also linear pyrrolic compounds including the **Sarcotrines** and **Sarcotragins** which are considered to have a common biosynthetic origin, the latter being degraded norsesterterpenoids.

Liu, Y. *et al.*, *Nat. Prod. Rep.*, 2006, **23**, 630–651 (*rev*)

DAPHNIPHYLLINE ALKALOIDS (VX6500)

The alkaloids of *Daphniphyllum* species constitute a unique group of complex bases derived from squalene. They are structurally diverse and a number of different numbering schemes have been used in the literature. The structures given in this Dictionary and their numbering have been revised to follow the scheme given by Kobayashi and Morita (2003), which is based on current knowledge about their biosynthesis. This system is based on various cyclisations of squalene-like intermediates, which have been modelled with success *in vitro*. The origin of the nitrogen atom is not certain; it may come from pyridoxamine or from an amino acid.



Daphniphylline

The first Edition of this Dictionary distinguished six structural subtypes of Daphniphyllum alkaloid. However, since new structural variations continue to be discovered regularly (e.g. **Bukittinggine**, **Calydaphninone**, containing a unique 4-membered ring), it is best to browse the individual entries or to consult the reviews listed below.

Yamamura, S., *Alkaloids*, 1986, **29**, 265–286 (*rev*)
Kobayashi, J. *et al.*, *Alkaloids*, 2003, **60**, 165–205 (*rev*, *biosynth*)
Jin, Z., *Nat. Prod. Rep.*, 2003, **20**, 608–614 (*rev*)

STEROIDAL ALKALOIDS (VX6640-VX6790)

The large number of steroidal alkaloids may be divided into several subgroups, of which the simplest are various types of aminopregnanes. Steroidal alkaloids are typically from higher plants, and are most numerous in the Apocynaceae, Liliaceae, Buxaceae and Solanaceae, however, some are from other sources, including amphibians.

A few naturally occurring steroidal aminoglycosides have been found (e.g. Holacurtinol), but these are not included in the Dictionary.

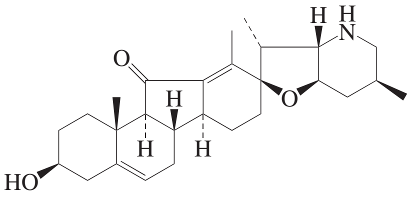
STEROIDAL ALKALOIDS (SALAMANDRA TYPE) (VX6640)

The small class of Salamandra-type alkaloids were isolated from amphibians, and are ring-A modified, mostly into aza-homosteroids, except for **Cycloneosamandione**.

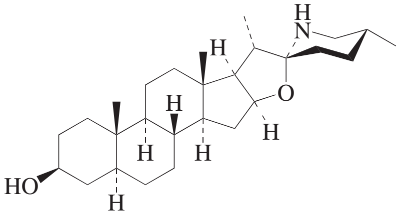
Habermehl, G., *Alkaloids*, 1967, **9**, 427–440 (*rev*)

STEROIDAL ALKALOIDS (JERVERATRUM, SPIROSOLANE AND SOLANIDINE TYPES) (VX6660, VX6720, VX6740)

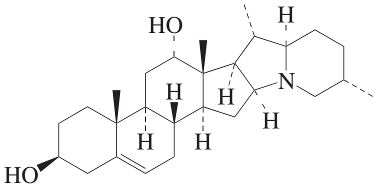
These are alkaloids in which the side-chain of a C_{27} steroid has been converted into a piperidine ring. In the jerveratrum (VX6660) (e.g. **Jervine**) and spirosolane (VX6720) (e.g. **Soladulcidine**) types, the piperidine ring is part of a spiro system, in the latter type forming an aza-analogue of the numerous and well- known spirostane steroids. Like the spirostanes, they show variation in the stereochemistry of the two new centres of chirality formed in the side-chain. In the solanidine type (VX6740), e.g. **Rubijervine**, an additional ring is formed by *C*-16 to *N* bond formation. They are present in the Solanaceae, and are of significance as potential trace toxins present in potatoes, tomatoes and other food crops.



Jervine



Soladulcidine

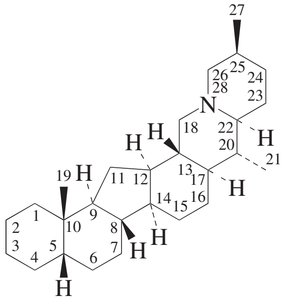


Rubijervine

Tomko, J. *et al.*, *Alkaloids*, 1973, **14**, 1–82 (*rev*)
Ripperger, H., *Alkaloids*, 1981, **19**, 81–192 (*rev*, *Solanum alkaloids*)
Ripperger, H. *et al.*, *Alkaloids Chem. Biol. Perspect.*, 1982, **12**, 103–186 (*rev*, *Solanum alkaloids*)
Keeler, R.F. *et al.*, *Alkaloids Chem. Biol. Perspect.*, 1986, **4**, 389–425 (*rev*, *teratogenic steroidal alkaloids*)

STEROIDAL ALKALOIDS (CERVERATRUM (CEVANE) TYPE) (VX6680)

In this group of alkaloids, from Monocot families such as the Orchidaceae, there has been an abeo shift from a Procevine-type precursor, in which ring D has been enlarged at the expense of ring C. They show extensive stereochemical variation within the basic cevane skeleton, and the stereochemistry of the various alkaloids is still being studied. See for example the numerous stereoisomers of **3,6-Cevanediol**.



Cevane (IUPAC)

The semisystematic nomenclature of cevanes, especially unsaturated ones, has shown some annoying minor variations over the years, e.g. Cev-5-enine, Cev-5-enene, Δ^5-Cevenine, 4,5-Didehydrocevane, etc. In this Dictionary the shortest form Cev-5-ene is used.

Ussuriedine represents an interesting tricyclic variation.

Tomko, J. *et al.*, *Alkaloids*, 1973, **14**, 1–82 (*rev*)

Steroidal alkaloids (conanine type) (VX6700)

Alkaloids containing the conanine skeleton occur in the Apocynaceae. Nearly all of these bases contain an amino or an oxygen function at *C*-3. There are some skeletal variations, such as *C*-4 methylation (**Kurcholessine**) and 9,10-seco-A ring aromatisation (**Didymeline**).

Atta-ur-Rahman *et al., Alkaloids*, 1988, **32**, 79–237 (*rev*)

Steroidal alkaloids (buxus type) (VX6760)

The *Buxus* alkaloids are a large group of bases, the majority of which are pentacyclic 4,4,14-trimethyl-9,19-cyclopregnanes. A smaller number contain a tetracyclic system in which 9,10 bond fission has occurred to give a seven-membered ring B. In some, one or both of the carbon atoms attached to *C*-4 have been lost. All the alkaloids have a nitrogen function at *C*-3 and/or *C*-20, which may be unmethylated, partially methylated, or fully methylated. Further minor structural variations continue to be isolated from various *Buxus* spp. The suffix letters used in the nomenclature of this group indicate the degree of methylation of the nitrogen atom(s):

In this Dictionary, the entries for these alkaloids are organised under the (usually unknown) unsubstituted parents of the I, O, or P type.

The recent characterisation of the **Cortistatin** alkaloids from a *Corticium* sponge, represent a new development. Structurally their $9(10\rightarrow19)$-abeosteroid moiety resembles that of one subgroup of the terrestrial *Buxus* alkaloids, but the presence of an isoquinoline ring system at the other end of the molecule is without precedent. They are coded as Buxus alkaloids on structural grounds, although presumably this is a case of evolutionary parallelism.

Černy, V. *et al., Alkaloids*, 1967, **9**, 305–426 (*rev*)
Tomko, J. *et al., Alkaloids*, 1973, **14**, 1–82 (*rev*)
Atta-ur-Rahman *et al., Alkaloids*, 1988, **32**, 79–237 (*rev*)
Ata, A. *et al., Alkaloids,* 2008, **66**, 191–213 (*rev*)

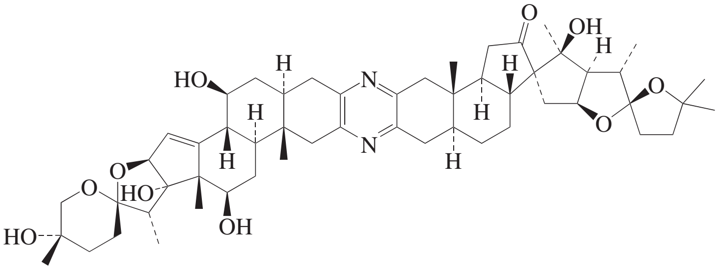
Steroidal alkaloids (pregnane type) (VX6780)

These are fairly numerous and occur in the Apocynaceae, Buxaceae and Didymelaceae. The majority contain amino or related functions at C-3 and/or C-20, and often at other positions.

Steroidal alkaloids (cephalostatins/ritterazines) (VX6785)

An important new group of marine steroidal metabolites isolated since the 1980s are the **Cephalostatins/Ritterazines**, which are dimeric steroidal pyrazines (also coded as pyrazine alkaloids). One of their representatives is **Ritterazine A**. They show significant biological activities, but are isolable only in small amounts and are the subject of intense synthetic efforts.

Flessner, T. *et al., Prog. Chem. Org. Nat. Prod.*, 2004, **87**, 1–80 (*rev*)



Ritterazine A

Miscellaneous steroidal alkaloids (VX6790)

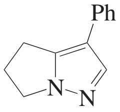
This includes non-nitrogenous steroids linked by an ester or acetal bond to a nitrogen containing unit, as in **Bufotoxin**, the **Batrachotoxins** (elaboration of a basic pregnane theme), and a small number of marine steroidal alkaloids of novel type such as the **Plakinamines**, as well as biologically active D-ring azahomosteroids based on **15-Azasterol**. **Petisidine**, **Tomatillidine** and their congeners are the only group of steroidal alkaloids containing a pyrrolidinyl side-chain. A 7-membered azepinyl ring structure was proposed for certain alkaloids such as **Edpetilidinine**, but most of these have now been reassigned as piperidines.

Azaanthracene and Azafluorene alkaloids (VX6820, VX6840)

There have been a number of structural reassignments in these groups, and some structures are still uncertain. It now appears that they are related to each other, and to the azaaporphine alkaloids (VX2830) above, via the azaanthraquinone intermediate as shown in the biosynthesis of Sampangine. They are therefore currently misplaced in the Type of Compound classification scheme.

Pyrazole alkaloids (VX6900)

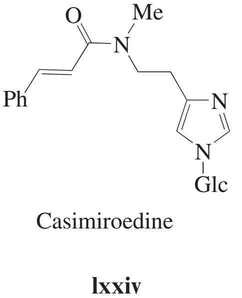
This is a small scattered group containing a few miscellaneous azapurine bases and simple hydrogenated pyrazoles. The most interesting alkaloid is **Withasomnine**. Little is known of its biosynthesis. Some early tracer studies showed incorporation of phenylalanine and ornithine, but at very low levels, and the significance of this is unclear. There is one marine example, **1-Methyl-1*H*-pyrazole-5-carboxylic acid**, from a gorgonian.



Withasomnine

Imidazole alkaloids (VX6920)

This group contains many structurally diverse examples, especially among marine and microbial alkaloids. There are various bases obviously containing a histamine moiety, e.g. **Casimiroedine**, and some more complex plant alkaloids. The bases isolated from marine sources include **Aplysinopsin** and related alkaloids and the **Rhopaladins**. They show a range of biological activities and considerable pharmaceutical potential. The most pharmacologically significant is **Pilocarpine**, obtainable only from *Pilocarpus* spp. (Rutaceae). Two possible biosynthetic pathways were suggested; the most probable involves condensation of a polyketide precursor of the lactone ring with a late intermediate in histidine biosynthesis as the source of the imidazole. This work of the 1970s does not appear to have been followed up more recently. **Anosmine** is biosynthesised from lysine.

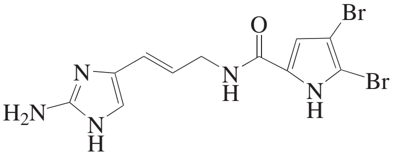


Casimiroedine

Hill, R.K., *Alkaloids Chem.Biol. Perspect.,Pelletier*, 1982, **2**, 49–104 (*rev*)
Maat, L. *et al., Alkaloids*, 1983, **22**, 282–334 (*rev*, *biosynth*)
Jin, Z. *et al.*, *Nat. Prod. Rep.*, 2006, **23**, 464–496 (*rev*)

PYRROLE-IMIDAZOLE ALKALOIDS (VX6922)

These form a varied class of marine alkaloid exemplified by **Oroidin** which with various relatives (e.g. the dimeric **Sceptrine**) appears to be a genuine sponge product. Their significance appears to be as key intermediates in the biogenesis of many of the more complex marine alkaloids. A recent biogenetically-based classification (see Hofmann) recognises a class of nearly 100 pyrrole-imidazole alkaloids arising in various ways from this key intermediate and containing 0-4 further rings, additional to the pyrrole and imidazole rings already present. Future organisation of this database may recognise this category; at present, many of these are placed in the miscellaneous categories VX9000–VX9400.

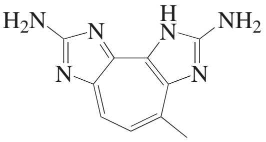


Oroidin

Hofmann, H. *et al.*, *Synthesis*, 2003, 1753–1783 (*rev*)
Walsh, C.T. *et al.*, *Nat. Prod. Rep.*, 2006, **23**, 577–531 (*rev*, *biosynth*)

CYCLOHEPTADIIMIDAZOLES (ZOANTHOXANTHINS) (VX6925)

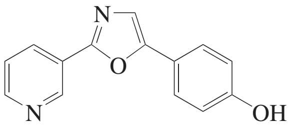
These are a group of marine alkaloids which are condensed imidazoles closely related in structure, and which in this Dictionary are grouped under just two entries; those for **Pseudozoanthoxanthin A** and **Parazoanthoxanthin A**. Their biosynthesis does not appear to have been studied in detail, however, they are presumably derived from histidine.



Pseudozoanthoxanthin A

OXAZOLE AND BENZOXAZOLE ALKALOIDS (VX6930)

Numerous naturally occurring oxazoles are known. Structurally they are diverse and may be open-chain (e.g. **Bengazoles**) or macrocyclic (e.g. **Patellamides**). Like the imidazoles, they show considerable drug potential. They have been isolated from various sources-plants of the Poaceae (e.g. **Annuloline**) and Rutaceae (e.g. **Halfordinol**), nudibranch egg masses (**Ulapualides**), algae and microorganisms. The latter have furnished the majority of the alkaloids, ranging from the simple indolyl alkaloids (**Pimprinine**) to complex peptide antibiotics such as the **Virginiamycin** family. The marine and bacterial oxazoles appear to have been formed from peptides of aliphatic amino acids, while the oxazoles of the Poaceae and Rutaceae arise from the chorismic acid-phenylalanine pathway.



Halfordinol

Jacobs, H.M. *et al., Alkaloids*, 1989, **35**, 259–310 (*rev*)
Pattenden, G., *J. Het. Chem.*, 1992, **29**, 607–618 (*rev*, *synth*)
Yeh, V.S.C., *Tetrahedron*, 2004, **60**, 11995–12042 (*rev*, *synth*)
Jin, Z. *et al.*, *Nat. Prod. Rep.*, 2006, **23**, 464–496 (*rev*)

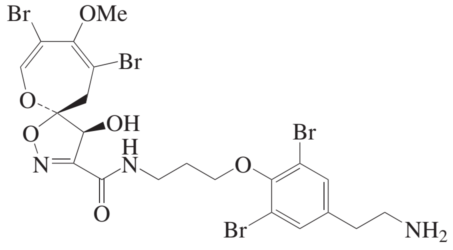
ISOXAZOLE ALKALOIDS (VX6932)

This is a fairly small group, most of which are modified amino acids (e.g. **Ibotenic acid**).

Rahboek, L. *et al., Alkaloids*, 2001, **57**, 185–233 (*rev*)

SPIROBENZOXAZOLINE ALKALOIDS (VX6934)

These exclusively marine alkaloids, such as the **Psammaplysins,** are derived by cyclisation of open-chain halogenated tyrosinoid oxime precursors (see VX2008 above). This is probably through the intermediacy of an arene oxide, although attempts to replicate this chemically have given only low yields.



Psammaplysin A

Okamoto, K.T. *et al.*, *Tet. Lett.*, 1987, **28**, 4969–4972 (*biosynth*)

THIAZOLE ALKALOIDS (VX6935, VX6936, VX6937)

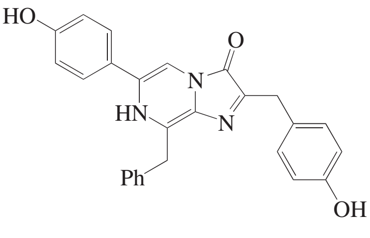
A large number of naturally occurring alkaloids that incorporate the thiazole nucleus have now been isolated. Some simple thiazoles (e.g. **2,4-Dialkylthiazoles**; **Benzothiazole**) have been obtained from plant and animal sources, but typically they are microbial products, including from marine sources. These alkaloids are a heterogeneous group ranging in complexity from **Aeruginoic acid** and the simple peptide **Herbamide A** to antineoplastic cyclopeptides such as **Ulicyclamide**, **Ulithiacyclamide**, **Patellamides** and **Dolastatins**. The **Latrunculins** (VX6936) are a subclass of mostly macrocyclic tetrahydrothiazoles isolated from sponges. Thiazoles show a range of interesting drug activities.

The biosynthesis of the thiazole ring in the highly bioactive **Curacin A** has been shown to be from cysteine, with the remainder of the carbon chain, including the cyclopropane functionality, being acetate-derived.

Pattenden, G., *J. Het. Chem.*, 1992, **29**, 607–618 (*rev, synth*)
Jin, Z. *et al.*, *Nat. Prod. Rep.*, 2005, **22**, 196–229; 2006, **23**, 464–496 (*revs*)
Mulzer, J., *Prog. Chem. Org. Nat. Prod.*, 2009, **90**, 1–237 (*Epothilones, rev, synth, biosynth, pharmacol*)

PYRAZINE AND QUINOXALINE ALKALOIDS (VX6940)

Pyrazines have been isolated from widely differing sources: from microorganisms, plants, mushrooms, animals, insects (especially ants, where they are considered to function as alarm pheromones) and various marine organisms, where they are the actual light emitters in bioluminescence processes. Bioluminescence emitters are found scattered throughout different types of organism, which implies multiple independent origins during the course of evolution. The imidazopyrazine, **Coelenterazine**, and closely related alkaloids though account for the great majority of observed bioluminescence. There is evidence for Coelenterazine *de novo* biosynthesis in shrimps. ***Cypridina* Luciferin** is biosynthesised from arginine and tryptophan. A series of tetrahydroquinoxalines has been isolated from the scent gland of the Canadian beaver, *Castor fiber*.



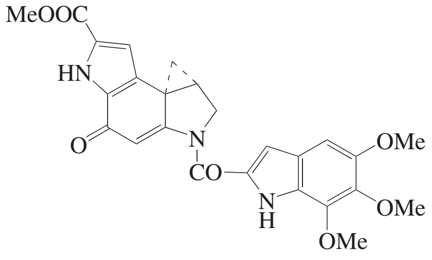
Coelenterazine

Pyrazines also contribute to the aroma of various foodstuffs, including coffee, cocoa, tea and cooked meats. However, from these sources they are generated by pyrolytic processes and are not true alkaloids. The cephalostatin group of alkaloids described under VX6785 are steroidal dimers linked by pyrazine formation.

Rees, J.-F. *et al.*, *J. Exp. Biol.*, 1998, **201**, 1211–1221 (*rev, bioluminescence*)

Benzo[1,2-*b*:3,4-*b*′]dipyrroles (VX6945)

This is a numerically limited group of alkaloid antibiotics all isolated from Streptomycetes. **Duocarmycin SA** appears to be a key biosynthetic intermediate, however, detailed biosynthetic studies have not been reported. They are DNA alkylating agents. Some members, e.g. **Rachelmycin**, are cyclopropa-compounds, however, this feature does not appear to be necessary for activity.



Duocarmycin SA

Pyrrolo[1,2-*a*]pyrazines (VX6950)

These are mostly cyclic anhydrides of proline plus another amino acid residue. Their inclusion in this Dictionary is a marginal decision. Other cyclodipeptides not based on proline are not included; they are classified under the amino acid code VV0150 (diketopiperazine) and are found in the *Dictionary of Natural Products*.

Morpholine alkaloids (VX6955)

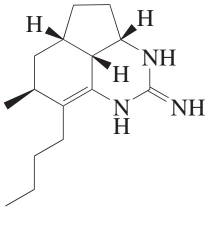
These are relatively few in number, e.g. **Agropine**, **Chelonins A** and **C** and the **Oxazinines**.

Pyrimidine alkaloids (VX6960)

Simple thymine-derived bases such as **Thyminol** are found in various organisms, together with some more highly elaborated substances such as the **Meridianins**. The category also includes miscellaneous hydrogenated pyrimidines, e.g. **Aberiamine**.

Ptilocaulins (VX6970)

This group is based on the (partially hydrogenated) cyclopenta[*de*]quinazoline skeleton, which contains a pyrimidine nucleus. It comprises **Ptilocaulin** and relatives, the **Mirabilins** and a few other related alkaloids, mostly isolated from sponges, but which may be symbiont metabolites. It has been suggested that these compounds arise by a late-stage addition of guanidine to a polyketide precursor.

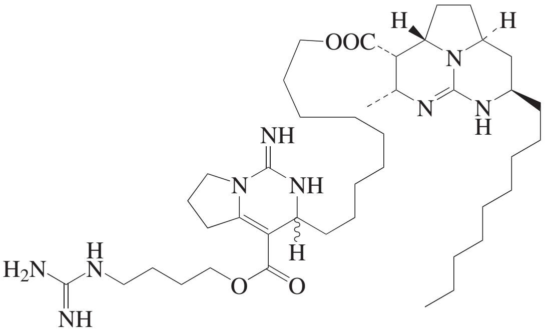


Ptilocaulin

Snider, B.B. et al., *J.Org.Chem*, 1993, **58**, 3828–3839 (*biosynth*)

Triazaacenaphthylene alkaloids (VX6980)

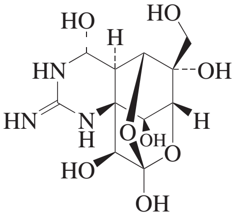
This is another group based on a tricyclic pyrimidine-related nucleus, and includes the **Batzelladines** and the **Crambescidins**. They are isolated from sponges and echinoderms. Their biosynthesis does not appear to have been studied in detail. However, they are formally composed of a guanidine unit, with which the biological activity is associated, embedded in a linear unbranched perimeter, presumably derived from a lipid precursor.



Batzelladine A

Tetrodotoxins (VX6990)

Tetrodotoxin and its homologues are well-known and important causes of human poisoning and are known principally from certain tissues of the Japanese puffer fish, and also found in other organisms; they are now thought to be *Pseudomonas* products. They have been extensively reviewed. The carbocycle ring in tetrodotoxins may be of isoprenoid origin.



Tetrodotoxin

Miyazawa, K. *et al., J. Toxicol., Toxin Rev.*, 2001, **20**, 11–25 (*rev*)
Yotsu-Yamashita, M., *J. Toxicol., Toxin Rev.*, 2001, **20**, 51–66 (*rev*)
Daly, J.W., *J. Nat. Prod.*, 2004, **67**, 1211–1215 (*rev, occur*)

Phenazine and phenoxazine alkaloids (VX7000, VX7005)

An increasing number of simple phenazines (e.g. the **Pelagiomicins**) and phenoxazines have been reported from microorganisms, including marine bacteria from sponges. There are also some more complex diphenazines such as **Saphenamycin** and the **Esmeraldines**. These, as well as the simpler phenazines, are biosynthesised by the shikimic acid pathway.

Van't Land, C.W. *et al., J. Org. Chem.*, 1993, **58**, 6576–6582 (*biosynth*)

Simple pyrrole alkaloids; miscellaneous pyrrole alkaloids (VX7010, VX7014)

The category VX7010 includes very simple brominated pyrroles (e.g. **2,3-Dibromo-1*H*-pyrrole**, which come from a variety of sources. Marine examples include the dimeric **Tambjamines**. Pyrrole-imidazole alkaloids are now listed above under VX6922, while the metabolically important tetrapyrroles, (chlorophyll, haem and their relatives) are not included in this Dictionary; consult the parent *Dictionary of Natural Products*. The pyrrole nucleus is a component of the indole alkaloids, but whereas these are tryptophan-derived, the polypyrroles are biosynthesised from 5-Amino-4-oxopentanoic acid (5-aminolaevulinic acid, ALA). Lower molecular weight alkaloids may arise from either route, or from proline/ornithine pathways via pyrrolidines (see above under VX0300); in the **Prodigiosins**, each of the three pyrrole residues is biosynthesised differently. The process of biohalogenation differs between Cl and Br. Chlorination takes place oxidatively by a combination of chloride ion, dioxygen and reduced FAD producing a Cl^+ equivalent, whilst bromination is mediated by vanadium bromoperoxidases.

LeQuesne, P.W. *et al., Alkaloids Chem. Biol. Perspect.*, 1999, **13**, 210–258, 237–288 (*revs*)
Gossauer, A., *Prog. Chem. Org. Nat. Prod.*, 2003, **86**, 1–188 (*rev*)
Berlinck, R.G.S., *Prog. Chem. Org. Nat. Prod..*, 2004, **87**, 2–188 (*rev*)
Walsh, C.T. *et al.*, *Nat. Prod. Rep.*, 2006, **23**, 517–531 (*rev*, *biosynth*)

POLYAMINE ALKALOIDS (VX7018, VX7020, VX7025, VX7050, VX7060, VX7080, VX7085, VX7090)

These categories cover the various types of alkaloid containing one or more -N(CH_2)$_n$N- groups, with *n* usually 3 or 4, less often 2 or 5. A useful subclassification scheme uses PA numbers defining the constituent diamine units, e.g. **Spermine** $H_2N(CH_2)_3NH(CH_2)_4NH(CH_2)_3NH_2$ is the parent substance of the PA343 subclass. They show markedly different properties (reactivity, basicity, complexing ability, mass spectrometry) from monobasic amines. Alkaloids based on the ornithine-derived **Putrescine** (PA4 alkaloids) (VX7020) are common in terrestrial plants where they are mostly simple cinnamoylputrescines, e.g. **Subaphylline**. Some have been characterised from marine organisms, such as the **Monodontamides** from gastropods. Numerous other alkaloids, again, many terrestrial and some marine, are derived from **Spermine** (PA343) (VX7080) or **Spermidine**, (PA34) (VX7050) themselves derived (in plants, certainly) from ornithine via putrescine. See for example the **Penaramides** and the unusual medium-ring azaaliphatic **Motuporamines**. Classes PA33, PA35, PA44 and PA33433 have also been found in nature, but less frequently. The largest number are the arachnid toxins, such as the extensive series of **Agel toxins** from the spider *Agelenopsis*. PA structures also occur in more complex alkaloids such as **Crambescidin 816** (PA34 substructure) and as steroidal conjugates, in **Squalamine** and related compounds from fish livers (PA34 and PA343 substructures). In terrestrial plants it is well established that these alkaloids derive from the decarboxylation and coupling of amino acids.

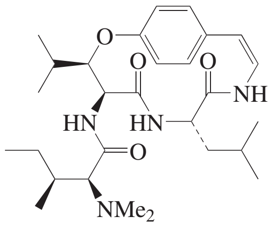
The spermidine group includes a variety of medium ring cyclic examples, e.g. **Codonocarpine**, **Lunaridine**, **Cannabisativine**. The PA44 class, the so-called homospermidine alkaloids, includes derivatives of the PA44 amine **Solamine** isolated from the Solanaceae.

Guggisberg, A. *et al., Alkaloids*, 1983, **22**, 85-188; 1997, **50**, 219–256 (*revs*)
Schafer, A. *et al., Alkaloids*, 1994, **45**, 1–125 (*arthropod toxins*)
Mueller, A.L. *et al., Alkaloids*, 1995, **46**, 63–94(*toxins*, *pharmacol*)
Bienz, S. *et al., Alkaloids*, 2002, **58**, 83–338 (*rev*)
Bienz, S., *Nat. Prod. Rep.*, 2005, **22**, 647–658 (*rev*)
Estrada, G., *Nat. Prod. Rep.*, 2007, **24**, 145–161 (*rev*, *spider toxins*)

ANSA-PEPTIDE ALKALOIDS (VX7100)

Peptides consisting only of unmodified proteinaceous amino acid chains, whether linear or cyclic, lie outside the scope of this Dictionary. Among the marine natural products there are a considerable number of peptide-like alkaloids containing highly modified residues, e.g. the Lissoclinamides. These are classified elsewhere (in the case of the Lissoclinamides, under VX6737, macrocyclic thiazole alkaloids).

A large class of peptide derivatives occurring exclusively in higher plants, particularly in the Rhamnaceae, are the ansa-peptide alkaloids, in which a medium-sized ring is formed by meta- or para-substitution of an aromatic peptide residue, as in **Frangulanine**. Many of these alkaloids incorporate D-amino acid residues, but the stereochemical information concerning them is sometimes incomplete. They have however been fully reviewed, with extensive tabulations.



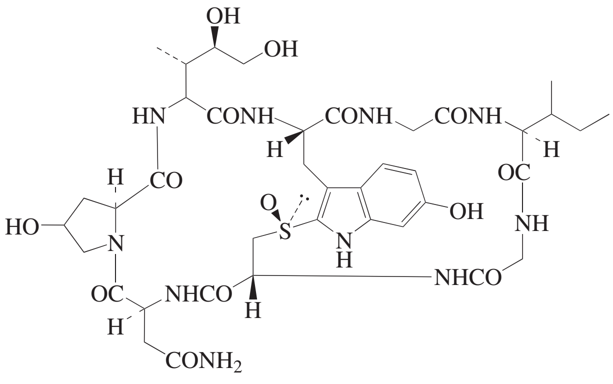
Frangulanine

Schmidt, U. *et al., Alkaloids*, 1985, **26**, 299–326 (*rev*)
Itokawa, H. *et al., Alkaloids*, 1997, **49**, 301–387 (*rev*)
Gournelis, D. *et al., Prog. Chem. Org. Nat. Prod.*, 1998, **75**, 1–180 (*rev*)

Tan, N.H. *et al., Chem. Rev*, 2006, **106**, 840–895 (*rev*)
El-Seedi, H., *et al., Phytochem. Rev.,* 2007, **6**, 143–165 (*rev*)

AMANITA ALKALOIDS (VX7120)

The toxins of the European death cap mushroom *Amanita phalloides* and other *Amanita* spp. constitute a complex group of macrocyclic peptides, mostly containing sulfur. These include the amatoxins (e.g. **α-Amanitin**, **β-Amanitin**), the phallotoxins (e.g. **Phalloidin**) and the virotoxins (e.g. **Viroidin**). They have been little studied recently apart from a new synthesis of Phalloidin.



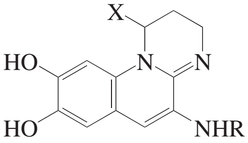
α-Amanitin

OTHER CYCLOPEPTIDE ALKALOIDS (VX7150)

This is a heterogeneous group.

PYOVERDINS (VX7170)

These are a fairly extensive and increasing series of peptide-alkaloidal siderophore pigments secreted by plant-growth promoting rhizobacteria *Pseudomonas* spp. under conditions of restricted iron availability. Their chelating properties protect the plant against attack by fungi and other pathogens by depriving them of iron. Although they were described in the nineteenth century, the first structure was not elucidated until 1981; by 1999 about 50 were known, some still with only partially determined structures.

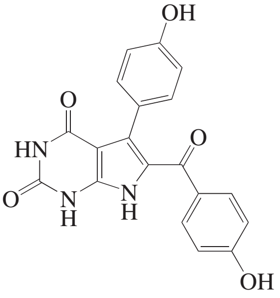


The chromophore is a pyrimido[1,2-*α*]quinoline system, sometimes modified as in the **Azotobactins**. The chromophoric properties of this heterocycle are associated with the predominance of a zwitterionic form having a positively charged quaternary nitrogen with delocalisation of charge over the two *N*s, but for clarity they are all shown in the Dictionary in the uncharged form. The chromophore is linked to a short nitrogenous substituent – NHR (R = usually a dioic acid, sometimes glycine) and an oligopeptide chain X, giving a typical total molecular weight of about 1000-1500. The peptide chain may be cyclic or acyclic, and may contain one or more unusual modified amino acid residues, such as 3-Amino-1-hydroxy-2-piperidinone (*N*-hydroxycycloornithine).
Caution; Compilation of Dictionary entries for this group has been complicated by inconsistencies in the literature concerning their structures and comparison with the molecular formulae, which are often not reported. Some inconsistencies remain in the Dictionary entries; checking continues.

Budzikiewicz, H., *Prog. Chem. Org. Nat. Prod.*, 2004, **87**, 81–237 (*rev*)

PYRROLO[2,3-*D*]PYRIMIDINE ALKALOIDS (VX7200)

This is a numerically limited group consisting of the nucleosides **Tubercidin**, the **Mycalisines** and related bases and some simple halogenated pyrrolopyrimidines, as well as the **Rigidins**. They have been isolated from marine organisms, and appear to be microbial products. It has been shown that the pyrimidine ring is derived intact from a purine base precursor which undergoes ring opening and reformation with the incorporation of a C_2 fragment to form the pyrrole ring.



Rigidin A

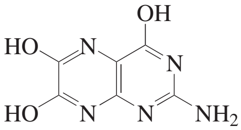
Purine alkaloids (VX7300)

Purines are involved along with pyrimidines as bases in DNA and RNA. The ubiquitous, well-known oxypurines, exemplified by **Caffeine**, are usually considered alkaloidal, alongside adenine derivatives such as the plant hormone, **Zeatin**; and various miscellaneous bases. The well-known purines, **Xanthine**, **Inosine**, **Theobromine** and **Theophylline**, long known as plant alkaloids, have now been found in marine organisms along with substituted purines (e.g. **Phidolopin**) and a range of terpenoid-purine alkaloids, such as the **Agelines** and others.

Rosemeyer, H., *Chem. Biodiversity*, 2004, **1**, 361–401 (*rev*)

Pteridine alkaloids (VX7350)

Pteridines are a widely distributed class of naturally occurring alkaloids. They owe their exceptional position in the field of heterocyclic chemistry mainly to their unusual chemical properties, their conspicuous fluorescence and their importance in metabolism, and partly to their discovery as pigments in butterfly wings. Three of the most common butterfly pigments are **Leucopterin**, **Xanthopterin** and **Isoxanthopterin**. The red pigments in the eye of the fruitfly *Drosophila melanogaster*, e.g. **Drosopterin**, **Isodrosopterin** and **Neodrosopterin** are more complex pteridines. **Folic acid**, a water-soluble growth factor in bacteria and an anti-pernicious anaemia factor in animals is also a pterin derivative with a *p*-aminobenzoylglutamic acid sidechain at the 6-position. It occurs naturally as the dihydro derivative. Marine pteridines are represented by **Leucettidine**, the **Urochordamines** and **Isoxanthopterin**.



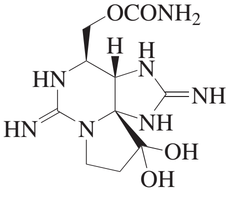
Leucopterin

The biosynthesis of pteridine pigments has been well studied in terrestrial organisms. As in the case of the pyrrolopyrimidines above, the imidazole ring is derived unchanged from a purine precursor, in this case guanosine triphosphate, and the pyrazine ring is built by ring fission and incorporation of two carbons derived from a ribose fragment.

Pfleiderer, W., *J. Het. Chem.*, 1992, **29**, 583–605 (*rev*)
Chemistry and Biology of Pteridines and Folates, (eds. Milstien, S. *et al.*), Kluwer, 2002

Saxitoxins (VX7400)

The saxitoxins are a group of highly important modified purinoid toxins known as Paralytic Shellfish Toxins or PSTs. Originally characterised as a cause of dangerous shellfish poisoning, they are now known to be biosynthesised only by dinoflagellates (and some freshwater cyanobacteria), although it is possible that the red alga *Jania* also produces them. Their presence in shellfish tissues probably results by diffusion according to a yet unknown mechanism. Their exact biosynthesis is not yet known, but it appears from radiolabelling experiments that the two guanidine groups derive from arginine and the carbamoyl side-chain from methionine.



Saxitoxin

Shimizu, Y., *Prog. Chem. Org. Nat. Prod.*, 1984, **45**, 235–264 (*rev*)
Garson, M.J., *Chem. Rev.*, 1993, **93**, 1699–1733 (*rev, biosynth*)
Llewellyn, L.E., *Nat. Prod. Rep.*, 2006, **23**, 200–222 (*rev*)

ALKALOIDAL METAL COMPLEXES (VX7450)

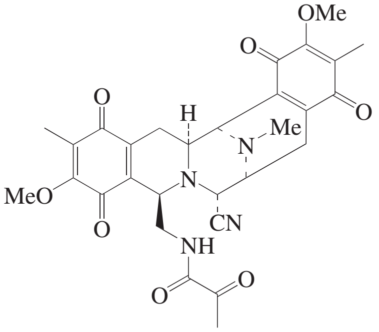
Alkaloidal chelates are additionally indexed here for ease of reference. The metals which have been identified so far in alkaloidal complexes are iron, copper, molybdenum and nickel.

NAPHTHYRIDINOMYCINS (VX7700)

This is a small group of microbial products, and labelling experiments have demonstrated the incorporation of tyrosine, ornithine and methionine.

SAFRAMYCINS (VX7800)

These are representative of the group known as the tetrahydroisoquinoline antitumour antibiotics, including some having slightly different skeletons, such as **Lemonomycin**. They are microbial products produced by *Streptomyces* spp. Close analogues such as the **Renieramycins** and the **Ecteinascidins** were isolated from marine organisms (sponges or tunicates) and are all presumably microbial products. The skeleton (studied for **Saframycin A**) is derived from two tyrosine molecules and the methyl groups from methionine.



Saframycin A

Arai, T. *et al., Alkaloids*, 1983, **21**, 56–100 (*rev*)
Murkami, Y. *et al.*, *J. Biol. Chem.*, 1985, **260**, 344–348 (*biosynth*)

MISCELLANEOUS ALKALOIDS WITH 0-4+ RINGS (VX9000, VX9100, VX9200, VX9300, VX9400)

These categories are self-explanatory. They include alkaloids whose relationships with the main groups has not been established, and individual alkaloids or small groups of alkaloids which are clearly related to one of the main groups, but which contain a modified carbon skeleton and are not numerous enough to merit special treatment.

ALKALOIDS OF UNKNOWN STRUCTURE (VX9999)

The Dictionary documents over 1000 alkaloids from the older literature where the structure has remained completely or partially undetermined. In cases where the Authors were able to propose a structural class for the

unknown isolate, the dictionary entry also carries the classification code relevant to that category, e.g. Buxus alkaloid.
Many of these isolates will remain forever unidentified, because the original sample is no longer available and the properties reported in the literature are not precise enough for a definite identification. Others, especially from the early literature, were doubtless ill-defined mixtures. However, the number of reinvestigations of these old isolations on a year-by-year basis is now surprisingly small, and renewed investigation of certain groups, for example the Amaryllidaceae alkaloids, using modern methods would probably yield interesting results.

6. DATABASE UPDATES

The database from which this Dictionary is produced, and which is represented by the CD-ROM version, is a specially enhanced subset of the *Dictionary of Natural Products*. Updates to the alkaloid information are being continuously incorporated into the DNP database and released to DNP subscribers. New editions of the *Dictionary of Alkaloids* (probably electronic only) will be published at future intervals.

Subscription information for DNP is available from **e-reference@taylorandfrancis.com** and www.chemnetbase.com.

Any comments and suggestions for inclusion to DNP may be sent to:

The Editors, DNP
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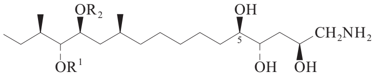
4th Floor, Albert House
1–4 Singer Street
London
EC2A 4BQ

AAL Toxin

A-1



TA_1 R^1 = H, R^2 = $COCH_2CH(COOH)CH_2COOH$
TA_2 R^1 = $COCH_2CH(COOH)CH_2COOH$, R^2 = H

Prod. by *Alternaria alternata* f. sp. *lycopersici*. Host-specific phytotoxin complex. Similar to Fumonisin A_1.

AAL Toxin TA_1 [79367-52-5]

$C_{25}H_{47}NO_{10}$ 521.647
Sol. H_2O.

5-Deoxy: ***AAL Toxin TB_1***
[149849-90-1]
$C_{25}H_{47}NO_9$ 505.648
From *Alternaria alternata* f. sp. *lycopersici*. Phytotoxin.

5-Deoxy, N-*Ac:* ***AAL Toxin TD_1***
[176590-35-5]
$C_{27}H_{49}NO_{10}$ 547.685

4,5-Dideoxy: ***AAL Toxin TC_1***
[176590-33-3]
$C_{25}H_{47}NO_8$ 489.648

4,5-Dideoxy, N-*Ac:* ***AAL Toxin TE_1***
[176590-37-7]
$C_{27}H_{49}NO_9$ 531.685

AAL Toxin TA_2 [79367-51-4]

$C_{25}H_{47}NO_{10}$ 521.647
Sol. H_2O.

5-Deoxy: ***AAL Toxin TB_2***
[149849-91-2]
$C_{25}H_{47}NO_9$ 505.648
From *Alternaria alternata* f. sp. *lycopersici*. Phytotoxin.

5-Deoxy, N-*Ac:* ***AAL Toxin TD_2***
[176590-36-6]
$C_{27}H_{49}NO_{10}$ 547.685

4,5-Dideoxy: ***AAL Toxin TC_2***
[176590-34-4]
$C_{25}H_{47}NO_8$ 489.648

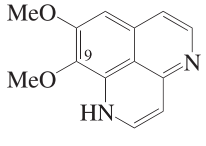
4,5-Dideoxy, N-*Ac:* ***AAL Toxin TE_2***
[176590-38-8]
$C_{27}H_{49}NO_9$ 531.685

Bottini, A.T. *et al., Tet. Lett.*, 1981, **22**, 2723 (*isol*)
Caldas, E.D. *et al., J. Agric. Food Chem.*, 1994, **42**, 327 (*struct*)
Boyle, C.D. *et al., J.A.C.S.*, 1994, **116**, 4995 (*struct*)
Oikawa, H. *et al., Tet. Lett.*, 1994, **35**, 1223 (*synth*)
Oikawa, H. *et al., Tetrahedron*, 1994, **50**, 13347 (*abs config*)
Shier, W.T. *et al., Tet. Lett.*, 1995, **36**, 1571 (*abs config*)
Oikawa, H. *et al., Tet. Lett.*, 1999, **40**, 6621-6625 (*synth, TA_1*)

Aaptamine

A-2

*8,9-Dimethoxy-1*H-*benzo[*de*][1,6]-naphthyridine, 9CI*
[85547-22-4]



$C_{13}H_{12}N_2O_2$ 228.25
Alkaloid from the marine sponge *Aaptos aaptos*. α-Adrenoreceptor blocker. Antineoplastic agent. Brilliant green cryst; bright yellow cryst. ($MeOH/Me_2CO$) (as hydrochloride). Sol. MeOH, $CHCl_3$. Mp 110-113° (107°) (hydrochloride). λ_{max} 215 (ε 13700); 236 (ε 14700); 255 (ε 17900); 309 (ε 3640); 350 (ε 3750); 380 (ε 5000); 394 (ε 4570) (H_2O) (Derep). λ_{max} 220 (ε 8900); 239 (ε 11750); 257 (ε 13200); 274 (ε 9700); 312 (ε 3160); 354 (ε 3300); 384 (ε 5620) (MeOH) (Berdy).

▶ DI2410500

N^4*-Me:* **N^4*-Methylaaptamine***
$C_{14}H_{14}N_2O_2$ 242.277
Alkaloid from *Aaptos aaptos*. Antiviral agent. Pale yellow oil. λ_{max} 216 (ε 1318); 239 (ε 13356); 258 (ε 11025); 269 (sh) (ε 9522); 277 (sh) (ε 8654); 314 (ε 2420); 360 (ε 2939); 394 (sh) (ε 2780) (MeOH).

O^9*-De-Me:* ***9-De-*****O*****-methylaaptamine***
[88839-98-9]
$C_{12}H_{10}N_2O_2$ 214.223
Alkaloid from *Aaptos aaptos*. Cytotoxic and antimicrobial agent. Greenish-yellow powder + $1.5H_2O$ (as hydrochloride). Mp 248-251° (dec., sealed tube) (hydrochloride). λ_{max} 241 (ε 18300); 313 (ε 3890); 370 (ε 4470); 400 (ε 4130) (H_2O) (Derep).

O^9*-De-Me,* N^1*-Me: 9-De-*O*-methyl-*N^1*-methylaaptamine.* ***Isoaaptamine***
[117173-75-8]
$C_{13}H_{12}N_2O_2$ 228.25
Alkaloid from the sponges *Aaptos aaptos*, *Hymeniacidon* sp. and *Suberites* sp. Antineoplastic agent and β-glucanase inhibitor. Amorph. yellow powder. Mp 200-205° dec.

*Di-*O*-de-Me:* ***Dide-*****O*****-methylaaptamine***
$C_{11}H_8N_2O_2$ 200.196
Isol. from *Aaptos* sp. Yellow solid (as TFA salt). λ_{max} 241 (log ε 4.43); 267 (log ε 4.19); 313 (log ε 3.63); 363 (log ε 3.67); 402 (log ε 3.58) (no solvent reported).

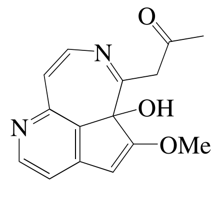
*Di-*O*-de-Me, 9-sulfate: Dide-*O*-methylaaptamine 9-sulfate*
$C_{11}H_8N_2O_5S$ 280.261
Isol. from *Aaptos* sp. Pale yellow solid (as TFA salt). λ_{max} 216 (log ε 4.14); 236 (log ε 4.12); 257 (log ε 4.18); 310 (log ε 3.49); 373 (log ε 3.63) (no solvent reported).

Nakamura, H. *et al., Tet. Lett.*, 1982, 5555 (*isol, uv, pmr, cmr, struct*)
Pelletier, J.C. *et al., Tet. Lett.*, 1985, **26**, 1259 (*synth, uv, pmr*)
Kelly, T.R. *et al., Tetrahedron*, 1985, **41**, 3033 (*synth*)
Sakamoto, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2760 (*synth*)
Bassoli, A. *et al., Chem. Comm.*, 1987, 150 (*synth*)
Nakamura, H. *et al., J.C.S. Perkin 1*, 1987, 173 (*deriv*)
Pelletier, J.C. *et al., J.O.C.*, 1987, **52**, 616 (*synth, ir, pmr*)
Andrew, R.G. *et al., Tetrahedron*, 1987, **43**, 4803 (*synth, uv, ir, pmr, ms*)
Hibino, S. *et al., J.C.S. Perkin 1*, 1988, 2429 (*synth, pmr*)
Fedoreev, S.A. *et al., Khim.-Farm. Zh.*, 1988, **22**, 943-946 (*isol*)
Sova, V.V. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 420-422 (*Demethyl-N-methylaaptamine*)
Balczewski, P. *et al., J.C.S. Perkin 1*, 1990, **31**, 3193 (*synth*)
Molina, P. *et al., Synthesis*, 1996, 1199 (*synth*)
Sugino, E. *et al., Heterocycles*, 1999, **50**, 543-559 (*rev, synth*)
Walz, A.J. *et al., J.O.C.*, 2000, **65**, 8001-8010 (*Isoaaptamine, synth*)
Coutinho, A.F. *et al., Heterocycles*, 2002, **57**, 1265-1272 (*N^4-Methylaaptamine*)
Calcul, L. *et al., Tetrahedron*, 2003, **59**, 6539-6544 (*isol, pmr, cmr*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2004, **67**, 506-509 (*Isoaaptamine, pmr, cmr, cryst struct*)
Pettit, G.R. *et al., J.O.C.*, 2004, **69**, 2251-2256 (*Isoaaptamine, synth*)
Herlt, A. *et al., Tetrahedron*, 2004, **60**, 6101-6104 (*Didemethylaaptamines*)
Larghi, E.L. *et al., Tetrahedron*, 2008, **64**, 5236-5245 (*synth*)

Aaptosamine

A-3

[219642-41-8]



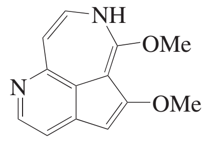
$C_{15}H_{14}N_2O_3$ 270.287
Alkaloid from the Red Sea sponge *Aaptos aaptos*. Orange gum. λ_{max} 240 (log ε 4.01); 336 (log ε 3.93) (MeOH).

Tinto, W.F. *et al., Heterocycles*, 1998, **48**, 2089-2093 (*isol, uv, ir, pmr, cmr, ms*)

Aaptosine

A-4

*1,9-Dimethoxy-8*H-*5,8-diazabenz[*cd*]azulene, 9CI*
[151041-63-3]



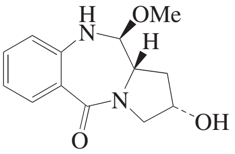
$C_{13}H_{12}N_2O_2$ 228.25
Trace alkaloid from the Red Sea sponge *Aaptos aaptos*. Cytotoxic agent. Yellow oil. λ_{max} 377 (MeOH/HCl) (Derep). λ_{max} 225 (ε 9700); 346 (ε 3800) (MeOH) (Derep).

Rudi, A. *et al., Tet. Lett.*, 1993, **34**, 4683 (*isol, uv, ir, pmr, cmr, ms, struct*)

Abbeymycin

A-5

*1,2,3,10,11,11*a*-Hexahydro-2-hydroxy-11-methoxy-5*H-*pyrrolo[2,1-*c*][1,4]benzodiazepin-5-one, 9CI. Antibiotic SA4-3. SA4-3*
[108073-64-9]
[115793-07-2]

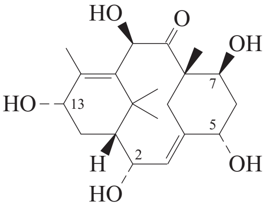


$C_{13}H_{16}N_2O_3$ 248.281
Anthramycin-type antibiotic from *Streptomyces* sp. Has weak activity against a limited number of anaerobic bacteria. Mp 142-144° dec. $[\alpha]_D^{25}$ +303 (c, 0.741 in H_2O). Stereochem. of SA4-3 not confirmed. λ_{max} 216 (ϵ 37200); 236 (ϵ 18100); 316 (ϵ 3600) (H_2O) (Derep).

▶ AA3000000

Hochlowski, J.E. *et al., J. Antibiot.*, 1987, **40**, 145 (*isol, uv, pmr, ms, struct*)
Japan. Pat., 1987, 87 185 087; *CA*, **109**, 92661m (*SA4-3*)

2(3→20)-Abeo-2,5,7,10,13-pentahydroxy-4(20),11-taxadien-9-one A-6



$C_{20}H_{30}O_6$ 366.453

(2α,5α,7β,10β,13α)-*form*

5-(3-Dimethylamino-3-phenylpropanoyl), 2,7,13-tri-Ac: [240805-52-1]
$C_{37}H_{49}NO_{10}$ 667.795
Constit. of *Taxus cuspidata*. Gum. $[\alpha]_D^{24}$ -31 (c, 0.01 in $CHCl_3$).

*5-(3*S*-Dimethylamino-2*S*-hydroxy-3-phenylpropanoyl), 13-Ac:* ***2-Deacetyltaxine A***. *Taxine C*
[160561-50-2]
$C_{33}H_{45}NO_9$ 599.72
Isol. from the leaves of *Taxus baccata* (Taxaceae). Amorph. or cryst. $[\alpha]_D^{20}$ -106 (c, 0.47 in $CHCl_3$).

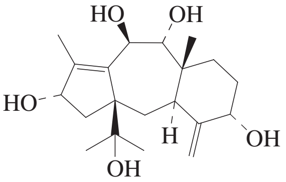
*5-(3*S*-Dimethylamino-2*S*-hydroxy-3-phenylpropanoyl), 2,13-di-Ac:* ***Taxine A***
[1361-49-5]
$C_{35}H_{47}NO_{10}$ 641.757
Major constit. of Taxine, the alkaloid mixt. from *Taxus baccata* (yew) (Taxaceae). Taxine is a common causal agent of cattle poisoning by *T.* spp. Cryst. (Me_2CO). Mp 204-206°. $[\alpha]_D$ -140 ($CHCl_3$).

*5-(3*S*-Dimethylamino-2*S*-hydroxy-3-phenylpropanoyl), 2,7,13-tri-Ac:* ***7-Acetyltaxine A***
[161956-28-1]
$C_{37}H_{49}NO_{11}$ 683.794
Constit. of *Taxus baccata*. Cryst. Mp 178-180°. $[\alpha]_D^{25}$ -96 (c, 1 in $CHCl_3$).

*5-(3*S*-Dimethylamino-2*S*-hydroxy-3-phenylpropanoyl), 2,7,10,13-tetra-Ac:* ***7,10-Diacetyltaxine A***
[244167-03-1]
$C_{39}H_{51}NO_{12}$ 725.831
Constit. of *Taxus yunnanensis*. Gum. $[\alpha]_D^{24}$ -75 (c, 0.01 in $CHCl_3$).

Graf, E. *et al., Annalen*, 1982, 376-381 (*Taxine A, cryst struct*)
Poupat, C. *et al., J. Nat. Prod.*, 1994, **57**, 1468-1469 (*2-Deacetyltaxine A*)
Barboni, L. *et al., Annalen*, 1995, 345-349 (*7-Acetyltaxine A, 2-Deacetyltaxine A*)
Shi, Q.-W. *et al., Tetrahedron*, 1999, **55**, 8365-8376 (*dimethylaminophenylpropanoyl tri-Ac*)

11(15→1)-Abeo-4(20),11-taxadiene-5,9,10,13,15-pentol A-7



$C_{20}H_{32}O_5$ 352.47

(5α,9α,10β,13α)-*form*

9-Ac: [153229-37-9]
$C_{22}H_{34}O_6$ 394.507
Constit. of *Taxus wallichiana*. Needles (MeOAc/hexane). Mp 160-162°. $[\alpha]_D^{20}$ -24 (c, 1.1 in MeOH). Struct. revised in 1993.

9,13-Di-Ac: [240805-50-9]
$C_{24}H_{36}O_7$ 436.544
Constit. of *Taxus yunnanensis*. Gum. $[\alpha]_D^{24}$ -17 (c, 0.01 in $CHCl_3$).

5,9,10,13-Tetra-Ac: [497879-22-8]
$C_{28}H_{40}O_9$ 520.619
Constit. of *Taxus wallichiana*. Oil. $[\alpha]_D^{20}$ +85 (MeOH).

5-Cinnamoyl, 9-Ac: [268728-61-6]
$C_{31}H_{40}O_7$ 524.653
Constit. of *Taxus yunnanensis*. Gum.

5E-*Cinnamoyl, 13-Ac:*
$C_{31}H_{40}O_7$ 524.653
Constit. of *Taxus yunnanensis*. Gum. $[\alpha]_D^{24}$ -17 (c, 0.01 in $CHCl_3$). λ_{max} 202 (ϵ 11700); 277 (ϵ 8400) (MeOH).

5-Cinnamoyl, 9,13-di-Ac: ***Chinentaxunine***
[260402-68-4]
[327024-58-8]
$C_{33}H_{42}O_8$ 566.69
Constit. of *Taxus chinensis*. Amorph. solid. $[\alpha]_D^{28}$ +43 (c, 0.49 in $CHCl_3$). $[\alpha]_D^{24}$ -23 (c, 0.01 in $CHCl_3$). λ_{max} 222 ; 277 (MeOH).

5-Cinnamoyl, 9,10,13-tri-Ac: ***7-Deacetoxytaxuspine J***
$C_{35}H_{44}O_9$ 608.727
Constit. of *Taxus cuspidata*. Amorph. solid. $[\alpha]_D^{20}$ -0.25 (c, 0.1 in MeOH). λ_{max} 202 (ϵ 11700); 277 (ϵ 8400) (MeOH).

5E-*Cinnamoyl, 10-benzoyl, 9,13-di-Ac:*
$C_{40}H_{46}O_9$ 670.798
Constit. of *Taxus yunnanensis*. Gum. $[\alpha]_D^{24}$ -11 (c, 0.01 in $CHCl_3$).

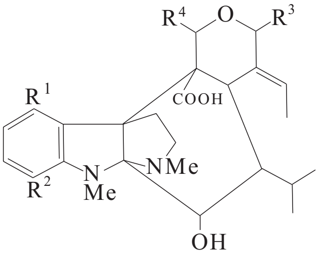
5-(3-Dimethylamino-3-phenylpropanoyl), 13-Ac: [260361-94-2]
$C_{33}H_{47}NO_7$ 569.737
Constit. of *Taxus yunnanensis*. Gum. $[\alpha]_D^{24}$ -27 (c, 0.01 in $CHCl_3$).

5-(3-Dimethylamino-3-phenylpropanoyl), 10-benzoyl, 9,13-di-Ac: [240805-51-0]
$C_{42}H_{53}NO_9$ 715.882
Constit. of *Taxus yunnanensis*. Gum. $[\alpha]_D^{24}$ -13 (c, 0.01 in $CHCl_3$).

Appendino, G. *et al., Chem. Comm.*, 1993, 1587-1589 (*struct*)
Barboni, L. *et al., Phytochemistry*, 1993, **33**, 145-150 (*9-Ac*)
Murakami, R. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1660-1663
Shi, Q.-W. *et al., J. Asian Nat. Prod. Res.*, 1999, **2**, 71-79; *CA*, **132**, 205456u (*deriv*)
Shen, Y.-C. *et al., Phytochemistry*, 1999, **52**, 1565-1569 (*Chinentaxunine*)
Shi, Q.-W *et al., Tetrahedron*, 1999, **55**, 8365-8376 (*isol, pmr, cmr*)
Shi, Q.-W. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 869-872 (*5-cinnamoyl-10-benzoyl-9,13-di-Ac*)
Shi, Q.W. *et al., Chin. Chem. Lett.*, 2000, **11**, 235-238 (*5-cinnamoyl-5-Ac*)
Shi, Q.-W. *et al., J. Asian Nat. Prod. Res.*, 2000, **2**, 311-319; *CA*, **134**, 190713r (*5-cinnamoyl-9,13-di-Ac*)
Kiyota, H. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 35-40 (*5-cinnamoyl-13-Ac*)
Choudhary, M.I. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1488-1490 (*5,9,10,13-tetra-Ac*)

Abereamine 1 A-8

[104386-96-1]



$R^1 = R^2 =$ OH, $R^3 = R^4 =$ H

$C_{25}H_{34}N_2O_6$ 458.553
Related to the Corymine/Isocorymine groups but with an additional isopropyl group the origin of which is not yet clear. Alkaloid from the seeds of *Hunteria umbellata* (Apocynaceae). Yellow solid. Sol. H_2O. Mp 199° dec.

Adegoke, E.A. *et al., Phytochemistry*, 1986, **25**, 1461-1468 (*isol, ir, pmr, ms, struct*)

Abereamine 2 A-9

[104406-77-1]
As Abereamine 1, A-8 with
$R^1 = R^3 =$ H, $R^2 = R^4 =$ OH
$C_{25}H_{34}N_2O_6$ 458.553
See note under Abereamine 1, A-8. Alkaloid from the seeds of *Hunteria umbellata* (Apocynaceae). Red solid. Sol. H_2O. Mp 230° dec.

Adegoke, E.A. *et al., Phytochemistry*, 1986, **25**, 1461-1468 (*isol, ir, pmr, ms, struct*)

Abereamine 3 A-10

[104386-97-2]
As Abereamine 1, A-8 with
$R^1 = R^2 =$ H, $R^3 = R^4 =$ OH
$C_{25}H_{34}N_2O_6$ 458.553
See note under Abereamine 1, A-8.

Alkaloid from the seeds of *Hunteria umbellata* (Apocynaceae). Brown solid. Sol. H_2O. Mp 280° dec.

Adegoke, E.A. *et al., Phytochemistry*, 1986, **25**, 1461-1468 (*isol, ir, pmr, cmr, ms, struct*)

Abereamine 4 A-11

[104386-98-3]

As Abereamine 1, A-8 with

$R^1 = R^4 = H, R^2 = R^3 = OH$

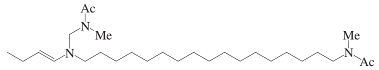
$C_{25}H_{34}N_2O_6$ 458.553

See note under Abereamine 1, A-8. Alkaloid from the seeds of *Hunteria umbellata* (Apocynaceae). Red solid. Sol. H_2O. Mp 260-262°.

Adegoke, E.A. *et al., Phytochemistry*, 1986, **25**, 1461-1468 (*isol, ir, pmr, ms, struct*)

Aberiamide A-12

[283167-82-8]



$C_{28}H_{55}N_3O_2$ 465.761

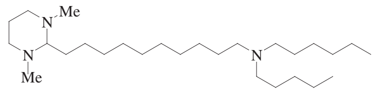
Alkaloid from the leaves of *Aberia caffra*. Pale yellow solid. $[\alpha]_D^{25}$ +20 (c, 1 in MeOH). Aberia is not a recognised genus (in the Kew system a synonym for *Dovyalis*).

Sayed, H.M. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 215-219 (*isol, pmr, cmr, ms*)

Aberiamine A-13

N-*Hexylhexahydro-1,3-dimethyl-*N-*pentyl-2-pyrimidinedecanamine, 9CI*

[283167-81-7]



$C_{27}H_{57}N_3$ 423.767

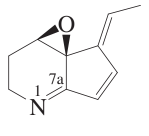
Alkaloid from the leaves of *Aberia caffra*. Pale yellow solid. $[\alpha]_D^{25}$ +3 (c, 1 in MeOH). Aberia is not a generally recognised genus (in the Kew system a synonym for *Dovyalis*).

Sayed, H.M. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 215-219 (*isol, pmr, cmr, ms*)

Abikoviromycin A-14

*7-Ethylidene-1*a*,2,3,7-tetrahydrocyclopent[*b*]oxireno[*c*]pyridine, 9CI, 8CI. 5-Ethylidene-4,4*a*-epoxy-2,3,4,4*a*-tetrahydro-1-pyrindene. Virocidin. SF 973A. Antibiotic SF 973A. Thomsomycin. Latumcidin*

[31774-33-1]



Absolute Configuration

$C_{10}H_{11}NO$ 161.203

Pyrindine numbering shown, for uniformity with other related compds. Prod. by *Streptomyces abikoensis, Streptomyces rubescens* and *Streptomyces latumcidicus*. Polyketide synthase inhibitor. Antifungal and antiviral agent. Highly unstable, polymerising on isol. from broth cultures. Can be handled in dilute soln. $[\alpha]_D^{21}$ +148.9 (c, 1 in 0.1*N* NaOH). λ_{max} 238 (ϵ 9980); 338 (ϵ 11600) (0.1*N* HCl) (Derep). λ_{max} 245 (ϵ 8690); 290 (ϵ 7730) (0.1*N* NaOH) (Derep). λ_{max} 243 (ϵ 9000); 289 (sh) (ϵ 8710); 345 (sh) (ϵ 4000) (EtOH or pH 7) (Derep). λ_{max} 244 (ϵ 13900) (MeOH) (Derep).

Sulfate: [43043-59-0]

Cryst. Mp 140-141° dec. $[\alpha]_D^{25}$ +24 (c, 1 in H_2O).

▶ GY8431000

Picrate:

Yellow needles (EtOAc/MeOH). Mp 136-137°.

*1,7*a*-Dihydro:* ***Dihydroabikoviromycin***. *Dihydrolatumcidin. Antibiotic SF 973B. SF 973B*

[20421-29-8]

$C_{10}H_{13}NO$ 163.219

Prod. by *Streptomyces olivaceus, Streptomyces viridochromogenes, Streptomyces reticuli* and *Streptomyces anulatus*. Mutagenic and genotoxic agent. Mp 60-61° (57-59°). $[\alpha]_D^{22}$ +276 (c, 1 in MeOH). pK_a 7.7 (50% EtOH aq.). pK_a 8.07. λ_{max} 244 (E1%/1cm 850) (MeOH) (Berdy).

*1,7*a*-Dihydro; hydrochloride:* Mp 130-132°.

*1,7*a*-Dihydro, 7-hydroxy:* ***Dihydro-*****N*****-hydroxyabikoviromycin***. N*-Hydroxydihydroabikoviromycin*

[109292-19-5]

$C_{10}H_{13}NO_2$ 179.218

From *Streptomyces* sp. SANK 65986. Exhibits antimicrobial activity. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 210 ; 242 (MeOH) (Berdy). λ_{max} 243 (MeOH-HCl) (Berdy). λ_{max} 210 ; 242 (MeOH-NaOH) (Berdy).

▶ LD_{50} (mus, ivn) 100 - 200 mg/kg.

Umezawa, H. *et al., Jpn. Med. J.*, 1951, **4**, 331; *CA*, **46**, 7167c (*isol*)

Sakagami, Y. *et al., J. Antibiot., Ser. A*, 1958, **11**, 6; 231; *CA*, **54**, 2483h; 2484a (*isol, uv, ir, struct*)

Gurevich, A.I. *et al., Tet. Lett.*, 1968, 2209 (*struct, pmr, ir, uv*)

Kono, Y. *et al., J. Antibiot.*, 1970, **23**, 572 (*pmr, cryst struct*)

Kono, Y. *et al., Acta Cryst. B*, 1971, **27**, 2341 (*cryst struct*)

Ogawa, Y. *et al., J. Antibiot.*, 1973, **26**, 186; 609 (*Dihydroabikoviromycin*)

Onda, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2916 (*isol, nmr, ms*)

Takahashi, S. *et al., Sankyo Kenkyusho Nenpo*, 1986, **38**, 105; *CA*, **107**, 55392n (*N-Hydroxydihydroabikoviromycin*)

Takahashi, S. *et al., CA*, 1987, **107**, 55392 (*deriv*)

Maruyama, H. *et al., J. Antibiot.*, 2003, **56**, 801-804 (*isol, pmr, cmr*)

Abrasine A-15

$C_{18}H_{21}N_3O_3$ 327.382

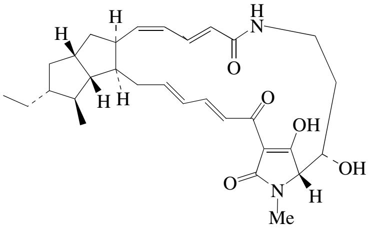
Struct. unknown. Alkaloid from roots of *Abrus precatorius* (Fabaceae). Mp 218-220° dec.

Hydrochloride: Mp 226-227°.

Khaleque, A. *et al., Sci. Res. (Dacca)*, 1966, **3**, 203-207; *CA*, **67**, 90987n (*isol, ir*)

Aburatubolactam A A-16

[170894-24-3]



$C_{30}H_{40}N_2O_5$ 508.656

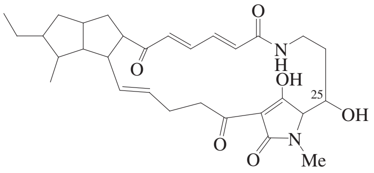
Tetramic acid deriv. Closely related to Alteramide A, A-661. Prod. by *Streptomyces* sp. SCRC-A20 from a marine mollusc. Cytotoxic agent, apoptosis inducer. Inhibitor of superoxide anion generation.

Japan. Pat., 1995, 95 228 583; *CA*, **123**, 337551v (*isol*)

Bae, M.-A *et al., Heterocycl. Commun.*, 1996, **2**, 315-318 (*isol, pmr, struct*)

Aburatubolactam B A-17

[170894-25-4]



$C_{30}H_{40}N_2O_6$ 524.656

Prod. by *Streptomyces* sp. SCRC A-20. Antiinflammatory and cytotoxic agent. Cryst. $[\alpha]_D$ +197 (Py).

25-Deoxy: ***Aburatubolactam C***

[170894-26-5]

$C_{30}H_{40}N_2O_5$ 508.656

Prod. by *Streptomyces* sp. SCRC A-20. Apoptosis-inducing substance. Antiinflammatory and cytotoxic agent. Powder. $[\alpha]_D$ +136 (Py).

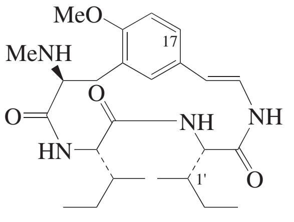
Japan. Pat., 1995, 95 228 583; *CA*, **123**, 337551v

Bae, M.-A. *et al., J. Microb. Biotechnol.*, 1998, **8**, 455-460

Abyssenine B A-18

Abyssinine B

[54519-15-2]



$C_{25}H_{38}N_4O_4$ 458.6

The alkaloids included in the entry need not necessarily have the same stereochem. Alkaloid from the bark of *Zizyphus abyssinica* and *Zizyphus mucronata* and from the stem bark of *Zizyphus oenoplia* (Rhamnaceae). Needles (MeOH/petrol). Mp 229-230°. $[\alpha]_D^{20}$ +151 (c, 0.16 in $CHCl_3$).

N-*De-Me:* ***Abyssenine C****. Abyssinine C*
[55857-03-9]
$C_{24}H_{36}N_4O_4$ 444.573
Alkaloid from the bark of *Zizyphus abyssinica* and from bark and leaves of *Zizyphus mucronata* (Rhamnaceae). Shows antibacterial and antifungal activity. Amorph. $[\alpha]_D^{20}$ +144 (c, 0.12 in $CHCl_3$). $[\alpha]_D^{20}$ -15 (c, 0.13 in MeOH).

17-Methoxy, N-*de-Me:* ***Mucronine G***
[55856-94-5]
$C_{25}H_{38}N_4O_5$ 474.599
Alkaloid from the bark and leaves of *Zizyphus mucronata* (Rhamnaceae). Amorph. $[\alpha]_D^{20}$ -50 (c, 0.084 in MeOH).

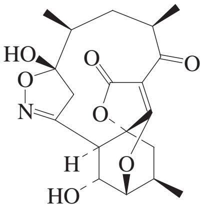
Z-*Isomer, 1′-hydroxy:* ***Zizyphine D***
[55323-68-7]
$C_{25}H_{38}N_4O_5$ 474.599
Alkaloid from the stem bark of *Zizyphus oenoplia* (Rhamnaceae). Needles (MeOH aq.). Mp 195°. $[\alpha]_D^{20}$ +236 (c, 0.10 in $CHCl_3$). $[\alpha]_D^{20}$ -121 (c, 0.10 in MeOH).

Z-*Isomer, 1′-hydroxy,* N-*de-Me:* ***Zizyphine E***
[55323-71-2]
$C_{24}H_{36}N_4O_5$ 460.572
Alkaloid from the stem bark of *Zizyphus oenoplia* (Rhamnaceae). Amorph. $[\alpha]_D^{20}$ +150 (c, 0.10 in $CHCl_3$). $[\alpha]_D^{20}$ -111 (c, 0.10 in MeOH).

Tschesche, R. *et al., Annalen*, 1974, 1915-1928 (*Abyssinines B,C, Mucronine G*)
Tschesche, R. *et al., Phytochemistry*, 1974, **13**, 2328 (*occur*)
Cassels, B.K. *et al., Tetrahedron*, 1974, **30**, 2461-2466 (*Abyssinine B, Zizyphines D,E*)
Hindenlang, D.M. *et al., Annalen*, 1980, 447 (*Zizyphine D, cmr*)
Wang, J. *et al., Tet. Lett.*, 2007, **48**, 6717-6721 (*synth, struct*)

Abyssomicin B A-19

[725254-08-0]



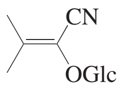
Absolute Configuration

$C_{19}H_{23}NO_7$ 377.393
Prod. by *Verrucosispora* sp. AB 18-032. Powder.

Bister, B. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 2574-2576 (*isol, struct*)
Riedlinger, J. *et al., J. Antibiot.*, 2004, **57**, 271-279 (*isol, activity*)

Acacipetalin A-20

2-(β-D-Glucopyranosyloxy)-3-methyl-2-butenenitrile, 9CI
[644-68-8]



$C_{11}H_{17}NO_6$ 259.258
Some confusion occurred in the literature around 1975. Isol. from *Acacia sieberiana* and *Acacia hebeclada*. Mp 177-179°. $[\alpha]_D^{26}$ -36.6 (H_2O).

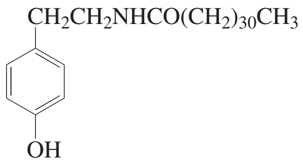
Tetra-Ac: [66890-86-6]
Mp 101-103°.

2,3-Dihydro: ***Dihydroacacipetalin***
$C_{11}H_{19}NO_6$ 261.274
Isol. from *Acacia sieberiana*.

Rimington, C. *et al., S. Afr. J. Sci.*, 1935, **32**, 154 (*isol*)
Ettlinger, M.G. *et al., Chem. Comm.*, 1977, 952 (*struct*)
Jaroszewski, J.W. *et al., Magn. Reson. Chem.*, 1987, **25**, 555 (*pmr, cmr*)

Acalyphamide A-21

N-*[2-(4-Hydroxyphenyl)ethyl]dotriacontanamide*
[81119-33-7]



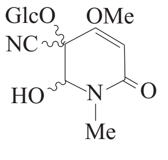
$C_{40}H_{73}NO_2$ 600.022
Isol. from *Acalypha indica*. Mp 135°.

Ac:
Amorph. solid ($CHCl_3$/MeOH). Mp 126°.

Talapatra, B. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 974

Acalyphin A-22

3-(β-D-Glucopyranosyloxy)-1,2,3,6-tetrahydro-2-hydroxy-4-methoxy-1-methyl-6-oxo-3-pyridinecarbonitrile, 9CI
[81861-72-5]

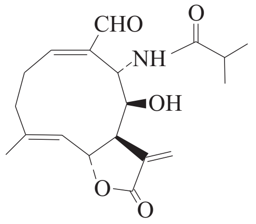


$C_{14}H_{20}N_2O_9$ 360.32
Alkaloid from the aerial parts of *Acalypha indica* (Euphorbiaceae). Also reported from Te Xian Cai (*Acalypha australis*) and *Acalypha farnesiana*. Hygroscopic powder. Mp 185-186° (182-184°). λ_{max} 223 (ϵ 6310); 255 (sh) (ϵ 2450) (EtOH) (Derep).

Nahrstedt, A. *et al., Phytochemistry*, 1982, **21**, 101 (*uv, ir, pmr, cmr, struct*)
Li, T.S.C. *et al., Chinese and Related North American Herbs*, CRC Press, 2002, 4 (*occur*)

Acanthamolide A-23

[64852-96-6]

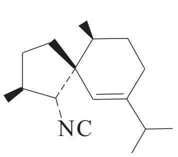


$C_{19}H_{25}NO_5$ 347.41
Constit. of *Acanthospermum glabratum*. Cryst. (C_6H_6/MeOH). Mp 249-251°. λ_{max} 225 (ϵ 10000) (MeOH) (Derep).

Saleh, A.A. *et al., J.C.S. Perkin 1*, 1980, 1090

Acanthisonitrile 3 A-24

[112766-99-1]



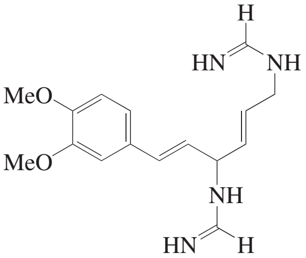
$C_{16}H_{25}N$ 231.38
Metab. of marine sponge *Acanthella acuta*. Oil. $[\alpha]_D$ -31.5 (c, 1.2 in $CHCl_3$).

Isothiocyanate: ***Acanthisothiocyanate 3***
[112767-00-7]
$C_{16}H_{25}NS$ 263.446
Metab. of *Acanthella acuta*. Oil. $[\alpha]_D$ -12.9 (c, 0.3 in $CHCl_3$). Has -NCS replacing -NC.

Mayol, L. *et al., Tetrahedron*, 1987, **43**, 5381-5388

Acanthoine A-25

N,N″*-[1-(3,4-Dimethoxystyryl)-2-butenylene]diformamidine, 8CI*
[6793-31-3]



$C_{16}H_{22}N_4O_2$ 302.375
Alkaloid from *Carduus acanthoides* (Asteraceae). Mp 221° (192-193°) (as dihydrochloride). $[\alpha]_D^{29}$ +7.1 (c, 0.4 in H_2O).

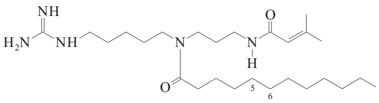
Tetrahydro: ***Acanthoidine****. Ruscopine*
[94347-15-6]
[4192-85-2]
$C_{16}H_{26}N_4O_2$ 306.407
Alkaloid from *Carduus acanthoides* (Asteraceae). Mp 250-251° (as hydrochloride). $[\alpha]_D^{22}$ +6.8 (c, 0.4 in H_2O). Saturated at both olefinic double bonds. The duplication of

trivial names is unexpected since both clearly refer to the same isol.

Frydman, B. *et al.*, *Tetrahedron*, 1962, **18**, 1063-1072 (*Acanthoine, Acanthoidine*)
U.S. Pat., 1964, 3 130 231; *CA*, **62**, 9188 (*synth*)
U.S. Pat., 1964, 3 130 230; *CA*, **61**, 3159 (*Ruscopine*)

3,5-Acarnidine **A-26**

$C_{12:0}$-Acarnidine
[67534-25-2]



$C_{26}H_{51}N_5O_2$ 465.721
Isol. from the sponge *Acarnus erithacus* as part of an inseparable mixt. Possesses broad antimicrobial activity and modest antiviral activity.

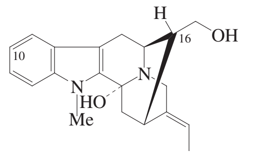
5,6Z-Didehydro: ***$C_{12:1}$-Acarnidine***
[67534-26-3]
$C_{26}H_{49}N_5O_2$ 463.705
Component of *Acarnus erithacus* acarnidine mixt. λ_{max} 218 (ϵ 17000) (no solvent reported) (Derep).

N-*Dedodecanoyl,* N-*(5Z,8Z,11Z-tetradecatrienoyl):* ***$C_{14:3}$-Acarnidine***
[67534-27-4]
$C_{28}H_{49}N_5O_2$ 487.727
Isol. from *Acarnus erithacus.*

Carter, G.T. *et al.*, *J.A.C.S.*, 1978, **100**, 4302-4304 (*isol, ir, pmr, cmr, ms, struct*)
Yorke, S.C. *et al.*, *Aust. J. Chem.*, 1986, **39**, 447-455 (*synth*)

Accedine **A-27**

1-Methylsarpagan-3,17-diol, 9CI
[58262-63-8]



Absolute Configuration

$C_{20}H_{24}N_2O_2$ 324.422
Alkaloid from *Tabernaemontana accedens* (Apocynaceae). Needles (MeOH). Mp 148-149°. $[\alpha]^{20}_{D}$ +72 (c, 0.096 in $CHCl_3$).

N-*De-Me:* ***Amerovolfine***. N-*Demethylaccedine*
[121312-84-3]
$C_{19}H_{22}N_2O_2$ 310.395
Alkaloid from the stem bark of *Rauwolfia tetraphylla* and *Rauwolfia cubana* (Apocynaceae). Needles (MeOH). Mp 183-184°. $[\alpha]^{20}_{D}$ +67 (c, 0.95 in MeOH).

N-*De-Me; hydrochloride:* Mp 280-282°.

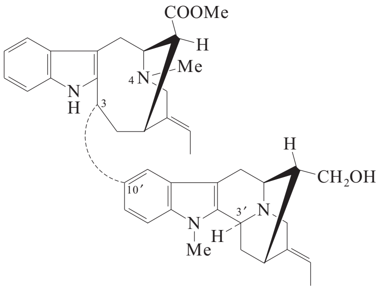
16-Epimer, N-*de-Me:* **N-Demethyl-16-epiaccedine**. *Sarpagan-3,7-diol, 9CI*
[59190-62-4]
$C_{19}H_{22}N_2O_2$ 310.395
Alkaloid from *Tabernaemontana accedens* (Apocynaceae). Mp 170-172°. $[\alpha]^{20}_{D}$ +50 (c, 0.06 in $CHCl_3$).

10-Hydroxy, N-*de-Me:* ***3-Hydroxysarpagine***
$C_{19}H_{22}N_2O_3$ 326.394
Alkaloid from the roots of *Rauwolfia serpentina*. Powder. $[\alpha]^{21}_{D}$ +44 (c, 1 in MeOH). λ_{max} 205 (log ϵ 4.36); 224 (log ϵ 4.23); 278 (log ϵ 3.75) (MeOH).

Achenbach, H. *et al.*, *Chem. Ber.*, 1975, **108**, 3842-3854 (*isol, uv, ir, pmr, ms, struct*)
Achenbach, H. *et al.*, *Tet. Lett.*, 1976, 351-352 (*N-Demethyl-16-epiaccedine*)
Martinez, J.A. *et al.*, *Phytochemistry*, 1989, **28**, 961-962 (*Amerovolfine*)
Martinez, J.A. *et al.*, *Planta Med.*, 1989, **55**, 283-285 (*Amerovolfine*)
Itoh, A. *et al.*, *J. Nat. Prod.*, 2005, **68**, 848-852 (*3-Hydroxysarpagine*)

Accedinisine **A-28**

Methyl 3-(17-hydroxy-1-methylsarpagan-10-yl)vobasan-17-oate, 9CI
[61551-76-6]



$C_{41}H_{48}N_4O_3$ 644.855
Alkaloid from *Tabernaemontana accedens* (Apocynaceae). Needles (Me_2CO). Mp 235° dec. $[\alpha]^{20}_{D}$ -60 (c, 0.4 in $CHCl_3$).

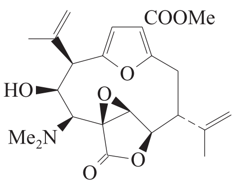
N^4*-De-Me:* ***Demethylaccedinisine***
[160427-83-8]
$C_{40}H_{46}N_4O_3$ 630.828
Alkaloid from stem bark of *Peschiera buchtieni* (Apocynaceae). Also a constit. of *Peschiera van heurkii*. $[\alpha]_D$ -30 (c, 0.3 in MeOH).

3′-Hydroxy: ***Accedinine***
[61551-77-7]
$C_{41}H_{48}N_4O_4$ 660.855
Alkaloid from *Tabernaemontana accedens* (Apocynaceae). Oil. $[\alpha]^{20}_{D}$ -81 (c, 0.2 in $CHCl_3$).

Achenbach, H. *et al.*, *Chem. Ber.*, 1976, **109**, 3527 (*isol, uv, ir, pmr, ms, struct, synth*)
Azoug, M. *et al.*, *Phytochemistry*, 1995, **39**, 1223 (*Demethylaccedinisine*)

Aceropterine **A-29**

[176227-10-4]



Relative configuration

$C_{23}H_{29}NO_7$ 431.485
Alkaloid from the Caribbean sea plume *Pseudopterogorgia acerosa*. $[\alpha]_D$ +0.44 (c, 2.0 in $CHCl_3$). Closely related to Tobagolide and Pseudopterolide. λ_{max} 258 (ϵ 3750) (MeOH) (Berdy).

Rodríguez, A.D. *et al.*, *Tet. Lett.*, 1996, **37**, 2687 (*isol, pmr, cmr, ms, struct*)

Acetamide, 9CI **A-30**

Ethanamide. Methanecarboxamide
[60-35-5]
H_3CCONH_2

C_2H_5NO 59.068
Isol. from some plants e.g. *Chimonanthus fragrans.* Produced industrially by distillation of ammonium acetate or by hydration of Acetonitrile. Solubiliser, plasticiser, stabiliser, used industrially as solv. in molten form. Dissolves virtually all classes of organic and inorganic compds. Deliquescent, hexagonal cryst. Odourless when pure but usually has characteristic "mouse" odour. V. sol. H_2O, EtOH; sol. $CHCl_3$; prac. insol. Et_2O. Mp 82-83°. Bp 222° Bp_5 92°. pK_{a1} -1.4 (25°). Triboluminescent.

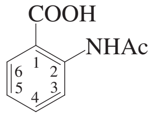
▶ Fl. p. >104°. Possible human carcinogen (IARC 2B). Irritant. Exp. carcinogen (v. large dose). Exp. reprod. and teratogenic effects (large doses). AB4025000

N-*(13-Methyltetradecyl):* ***Capsiamide***
[64317-66-4]
$C_{17}H_{35}NO$ 269.47
Constit. of fruit of hot pepper varieties of *Capsicum annuum.*

Takahashi, M. *et al.*, *Yakugaku Zasshi*, 1977, **97**, 758 (*Capsiamide*)
Speakman, J.C. *et al.*, *J. Chem. Res., Synop.*, 1979, 277 (*cryst struct*)
ul Hassan, M. *et al.*, *Org. Magn. Reson.*, 1980, **14**, 447 (*cmr*)
Gonzalez, G. *et al.*, *J.C.S. Faraday 2*, 1981, 2231 (*pmr*)
Kerridge, D.H. *et al.*, *Chem. Soc. Rev.*, 1988, **17**, 181 (***rev***)
Liu, L.K. *et al.*, *Acta Cryst. C*, 1994, **50**, 1333 (*cryst struct, hydrochloride*)

2-Acetamidobenzoic acid **A-31**

2-(Acetylamino)benzoic acid, 9CI. N-*Acetylanthranilic acid. Lappaconitic acid*
[89-52-1]



$C_9H_9NO_3$ 179.175
Needles (AcOH). Mp 185°. pK_a 5.64.

▶ LD_{50} (mus, orl) 1114 mg/kg. CB2455000

Me ester: [2719-08-6]
$C_{10}H_{11}NO_3$ 193.202
Needles (EtOH). Mp 101°.

Et ester: [20628-20-0]
$C_{11}H_{13}NO_3$ 207.229
Needles (EtOH). Mp 64-65°.

Amide: 2-Acetamidobenzamide. 2-(Acetylamino)benzamide. ***Antibiotic NP 101A***. *NP 101A*
[33809-77-7]
$C_9H_{10}N_2O_2$ 178.19
Prod. by *Streptomyces aurantiogriseus* and *Cytophaga marinoflava* sp. AM13.1. Antifungal agent. Needles

(EtOH). Sol. MeOH, EtOH, EtOAc, C_6H_6, DMSO, Py; poorly sol. H_2O. Mp 179-180° (α-form) Mp 189-190° (β-form). Exists in two cryst. forms, accounting for unreliable melting point determinations. λ_{max} 219 (log ϵ 3.56); 252 (log ϵ 3.31); 299 (log ϵ 2.72) (MeOH). λ_{max} 219 (ϵ 3630); 252 (ϵ 2042); 299 (ϵ 550) (MeOH) (Berdy).

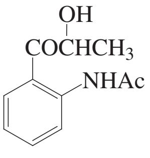
▶CU8702020

N-*Ac: Diacetylanthranilic acid*
$C_{11}H_{11}NO_4$ 221.212
Prisms (EtOH). Mp 180°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 356D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1362B (*nmr*)
Matsuo, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 990 (*nmr*)
Erikson, J. *et al., J. Chem. Educ.*, 1972, **49**, 688 (*synth*)
Matsuda, V. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 430 (*synth*)
Ger. Pat., 1976, 2 556 590; *CA*, **85**, 160115 (*synth*)
Errede, L.A. *et al., J.C.S. Perkin 2*, 1981, 233-238 (*Acetamidobenzamide*)
Phay, N. *et al., J. Antibiot.*, 1996, **49**, 703-705 (*Acetamidobenzamide*)
Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*Cytophaga marinoflava isol*)
Kelleher, J.M. *et al., ARKIVOC*, 2007, **xvi**, 209-226 (*Acetamidobenzamide, powder struct, polymorphism*)

1-(2-Acetamidophenyl)-2-hydroxy-1-propanone A-32

N-*[2-(2-Hydroxy-1-oxopropyl)phenyl]acetamide, 9CI. 2-(2-Hydroxypropanoyl)acetanilide*
[150641-66-0]



$C_{11}H_{13}NO_3$ 207.229
Prod. by *Nocardia* sp. DSM 43130. $[\alpha]_D$ -8 ($CHCl_3$). λ_{max} 217 ; 253 ; 339 (MeOH). λ_{max} 217 ; 253 ; 339 (MeOH) (Berdy).

Abraham, W.R. *et al., Phytochemistry*, 1993, **33**, 929-930

2-[(2-Acetamidopropanoyl)amino]benzamide A-33

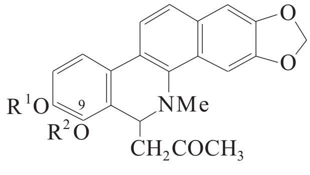
N^2-*[2-(Acetylamino)propanoyl]anthranilamide.* N^2-*Acetylalanylanthranilamide*
$C_{12}H_{15}N_3O_3$ 249.269

(S)-*form*
Antibiotic NI 15501A. *NI 15501A*
[208345-44-2]
Prod. by the marine fungus *Penicillium* sp. NI15501. Solid. Sol. MeOH, butanol; poorly sol. H_2O. $[\alpha]_D^{30}$ -62.8 (c, 0.15 in MeOH). λ_{max} 216 (ϵ 12000); 253 (ϵ 6100); 290 (ϵ 1800) (MeOH).

Onuki, H. *et al., J. Antibiot.*, 1998, **51**, 442-444 (*isol, uv, ir, pmr, cmr, ms*)

8-Acetonyldihydrochelerythrine A-34

12,13-Dihydro-1,2-dimethoxy-12-methyl-13-(2-oxopropyl)-1,3-benzodioxolo[5,6-c]phenanthridine, 9CI. 13-Acetonyl-12,13-dihydrochelerythrine, 8CI. 11-Acetonyldihydrochelerythrine. Alkaloid ZT$_1$. 6-Acetonyldihydrochelerythrine
[22864-92-2]



$R^1 = R^2 = Me$

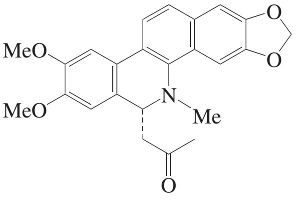
$C_{24}H_{23}NO_5$ 405.449
Probably an artifact. Numbering systems vary. Alkaloid from the root bark of *Toddalia aculeata* and *Xylocarpus granatum*, and from the bark of *Zanthoxylum conspersipunctatum* and *Zanthoxylum tsihanimposa* (Rutaceae, Meliaceae). Also obt. by the base-catalysed addn. of acetone to Chelerythrine. Plates (Me_2CO). Mp 199° (190-192°, 194-195°). λ_{max} 228 (log ϵ 4.52); 283 (log ϵ 4.61); 320 (log ϵ 4.18) (solvent not reported).

O^9-*De-Me:* O-*Desmethyldihydrochelerithrinyl-8-acetone.* O-*Desmethyldihydrochelerithrinyl-11-acetone. Alkaloid ZT$_3$*
[51888-34-7]
$C_{23}H_{21}NO_5$ 391.423
Isol. from the bark of *Zanthoxylum tsihanimposa* (Rutaceae). Cryst. (MeOH). Mp 201-205°. Opt. inactive, prob. an artifact. λ_{max} 229 (log ϵ 4.55); 284 (log ϵ 4.62); 320 (log ϵ 4.17) (EtOH). λ_{max} 234 (log ϵ 4.48); 297 (log ϵ 4.52); 338 (log ϵ 4.33) (EtOH + NaOH).

Desai, P.D. *et al., Indian J. Chem.*, 1967, **5**, 41-42 (*uv, ir, pmr, ms, struct*)
MacLean, D.B. *et al., Can. J. Chem.*, 1969, **47**, 1951-1956 (*synth, ir, pmr, ms*)
Corrie, J.E.T. *et al., Aust. J. Chem.*, 1970, **23**, 133-145 (*synth, uv, ir, ms*)
Krajniak, E.R. *et al., Aust. J. Chem.*, 1973, **26**, 687-689 (*isol*)
Decaudain, N. *et al., Phytochemistry*, 1974, **13**, 505-511 (*O^9-de-Me*)
Chou, F.Y. *et al., Heterocycles*, 1977, **7**, 969-975 (*occur*)
Sharma, P.N. *et al., Phytochemistry*, 1981, **20**, 2781-2783 (*isol*)

8-Acetonyldihydronitidine A-35

[80330-39-8]



Relative Configuration

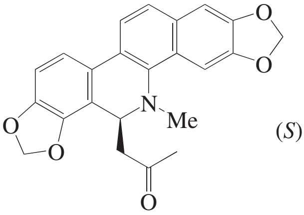
$C_{24}H_{23}NO_5$ 405.449
Alkaloid from the stem bark of *Zanthoxylum tetraspermum*. Antibacterial agent. Cryst. Mp 165-167°. $[\alpha]_D$ 0 ($CHCl_3$). λ_{max} 316 (log ϵ 3.87) (EtOH).

*10,11-Di-*O*-de-Me, 10,11-methylene ether:* ***8-Acetonyldihydroavicine***
[348098-59-9]
$C_{23}H_{19}NO_5$ 389.407
Alkaloid from the stem bark of *Zanthoxylum tetraspermum*. Antibacterial agent. Cryst. Mp 184-185°. $[\alpha]_D^{25}$ -6.6 ($CHCl_3$). λ_{max} 321 (log ϵ 4.2) (EtOH).

Nissanka, A.P.K. *et al., Phytochemistry*, 2001, **56**, 857-861 (*isol, pmr, cmr, 8-Acetonyldihydroavicine*)
Morel, A.F. *et al., Acta Cryst. C*, 2002, **58**, 606-607 (*Acetonyldihydroavicine, cryst struct*)
Wang, X.-L. *et al., Acta Cryst. E*, 2006, **62**, 2247-2248 (*cryst struct*)

8-Acetonyldihydrosanguinarine A-36

6-Acetonylsanguinarine. 6-Acetonyldihydrosanguinarine
[37687-34-6]



(*S*)-*form*

$C_{23}H_{19}NO_5$ 389.407

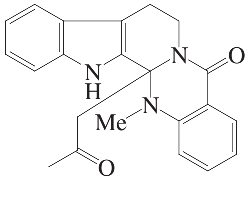
(*S*)-*form*
Alkaloid from the roots of *Corydalis flabellata*. Needles ($CHCl_3$/EtOH). Mp 209-210°. $[\alpha]_D^{20}$ +25.3 (c, 0.02 in $CHCl_3$). λ_{max} 232 (log ϵ 4.4); 282 (log ϵ 4.6); 323 (log ϵ 4.8) ($CHCl_3$).

(ξ)-*form*
Alkaloid from *Argemone mexicana*, the callus tissue of *Papaver somniferum* (opium poppy) and the roots of *Glaucium flavum* var. *vestitum* (Papaveraceae). Also obt. by the base-catalysed condensation of sanguinarine with acetone. Pale yellow needles (MeOH/$CHCl_3$). Mp 194-195.5°.

Furuya, T. *et al., Phytochemistry*, 1972, **11**, 3041-3044 (*isol, uv, ir, pmr, ms, struct, synth*)
Döpke, W. *et al., Z. Chem.*, 1976, **16**, 54-55 (*occur, uv, ir, pmr, ms, struct*)
Castedo, L. *et al., Heterocycles*, 1981, **16**, 533-536 (*occur*)
Koul, S. *et al., Planta Med.*, 2002, **68**, 262-265 (*isol, pmr, cmr, ms*)

Acetonylevodiamine A-37

[848601-89-8]

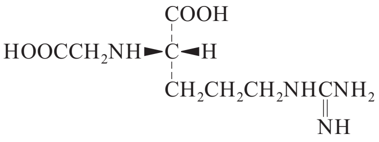


$C_{22}H_{21}N_3O_2$ 359.427
Alkaloid from the fruit of *Evodia rutaecarpa*. Mp 163-164°.

Zuo, G.Y. *et al., Yunnan Zhiwu Yanjiu*, 2003, **25**, 103-106; *CA*, **142**, 332872h (*isol*)

Acetopine A-38

N^2*-(Carboxymethyl)arginine, 9CI. Demethyloctopine*



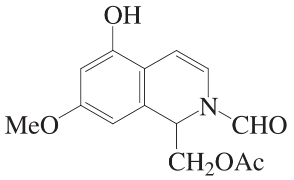
$$HOOCCH_2NH\blacktriangleright\overset{COOH}{\underset{CH_2CH_2CH_2NHC(=NH)NH_2}{C}}\blacktriangleleft H$$

$C_8H_{16}N_4O_4$ 232.239

(S)-form
L-form
[18416-86-9]
Isol. from cotton (*Gossypium hirsutum*) and soybean (*Glycine max*) callus. Cryst. (EtOH aq.). Mp 281-282°. $[\alpha]_D^{24}$ +24 (c, 2.5 in H_2O).

Herbst, R.M. *et al., J.O.C.*, 1946, **11**, 368 (*synth*)
Christou, P. *et al., Plant Physiol.*, 1986, **82**, 218 (*isol*)

1-(Acetoxymethyl)-2-formyl-1,2-dihydro-5-hydroxy-7-methoxyisoquinoline A-39



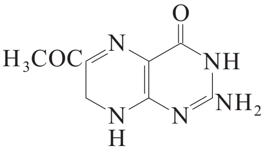
$C_{14}H_{15}NO_5$ 277.276

(+)-form
Alkaloid from the sponge *Petrosia similis*. Amorph. solid. $[\alpha]_D^{25}$ +208 (c, 0.72 in $CHCl_3$). λ_{max} 224 (ϵ 6660); 228 (ϵ 6680); 231 (ϵ 6650); 299 (ϵ 4790) (MeOH).

Ramesh, P. *et al., J. Nat. Prod.*, 1999, **62**, 780-781 (*isol, uv, pmr, cmr, ms*)

6-Acetyl-2-amino-7,8-dihydro-4(3*H*)-pteridinone, 9CI A-40

Sepiapterin C
[42310-08-7]

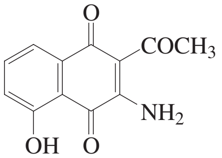


$C_8H_9N_5O_2$ 207.191
Pigment from *Drosophila melanogaster*. Yellow cryst. (H_2O).

Sugiuva, K. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3312 (*isol, struct*)

2-Acetyl-3-amino-5-hydroxy-1,4-naphthoquinone A-41

2-Acetyl-3-amino-5-hydroxy-1,4-naphthalenedione, 9CI

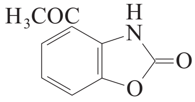


$C_{12}H_9NO_4$ 231.207
Constit. of the stem bark of *Goniothalamus marcanii*. Yellow powder. λ_{max} 260 (log ϵ 4.31); 296 (log ϵ 4.08) (MeOH).

Soonthornchareonnon, N. *et al., J. Nat. Prod.*, 1999, **62**, 1390-1394

4-Acetyl-2(3*H*)-benzoxazolone, 9CI A-42

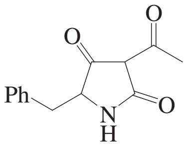
4-Acetylbenzoxazolin-2-one
[70735-79-4]



$C_9H_7NO_3$ 177.159
Found in kernels of *Zea mays* (sweet corn) (Poaceae). Needles (Me_2CO aq.). Mp 217-218°. λ_{max} 250 (ϵ 9777); 320 (ϵ 5128) (MeOH) (Berdy). λ_{max} 268 (ϵ 8912); 351 (ϵ 7413) (MeOH/NaOH) (Berdy).

Fielder, D.A. *et al., Tet. Lett.*, 1994, **35**, 521-524 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Fielder, D.A. *et al., J. Nat. Prod.*, 1995, **58**, 456-458 (*synth*)
Escobar, C.A. *et al., J. Het. Chem.*, 1997, **34**, 1407-1414 (*synth*)
Kluge, M. *et al., J. Nat. Prod.*, 1998, **61**, 821-822 (*synth*)

3-Acetyl-5-benzyl-2,4-pyrrolidinedione A-43

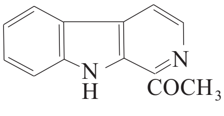


$C_{13}H_{13}NO_3$ 231.251
Enolised β-tricarbonyl compd. with several tautomers possible. Isol. from *Leocarpus fragilis*. No phys. props. reported.

Steglich, W. *et al., Pure Appl. Chem.*, 1989, **61**, 281-288

1-Acetyl-β-carboline A-44

*1-(9*H*-Pyrido[3,4-*b*]indol-1-yl)ethanone, 9CI*
[50892-83-6]



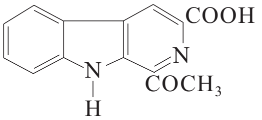
$C_{13}H_{10}N_2O$ 210.235
The compd. lycii Alkaloid I, isol. from several plant spp. and erroneously assigned the struct. N^9-Formylharman, has now been shown by Bracher *et al* to be identical with 1-Acetyl-β-carboline. Alkaloid from the bark of *Ailanthus malabarica* (Simaroubaceae). Also isol. from the sponge *Tedania ignis*. Light yellow solid. Mp 203-205°.

N^2*-Oxide:*
$C_{13}H_{10}N_2O_2$ 226.234
Mp 180°.

Joshi, B.S. *et al., Heterocycles*, 1977, **7**, 193 (*isol, uv, ir, pmr, ms, struct*)
Dillman, R.L. *et al., J. Nat. Prod.*, 1991, **54**, 1056-1061; 1141 (*isol, sponge, ir, pmr, cmr, ms*)
Bracher, F. *et al., Annalen*, 1993, 837; 1335 (*synth, pmr, cmr, lycii Alkaloid I*)
Bracher, F. *et al., Synth. Commun.*, 1995, **25**, 1557 (*synth*)
Zhou, T.-S. *et al., Phytochemistry*, 1998, **49**, 1807-1809 (*isol, uv, ir, pmr, cmr*)
Kast, O. *et al., Synth. Commun.*, 2003, **33**, 3843-3850 (*N^2-oxide*)

1-Acetyl-β-carboline-3-carboxylic acid A-45

*1-Acetyl-9*H*-pyrido[3,4-*b*]indole-3-carboxylic acid, 9CI. 1-Acetyl-3-carboxy-β-carboline*
[73818-29-8]



$C_{14}H_{10}N_2O_3$ 254.245
Alkaloid from aerial parts of *Vestia lycioides* (Solanaceae). Mp 347-350°.

Me ester: ***1-Acetyl-3-methoxycarbonyl-β-carboline***
[66154-37-8]
$C_{15}H_{12}N_2O_3$ 268.271
Alkaloid from *Vestia lycioides* (Solanaceae). Yellow needles ($CHCl_3$/MeOH). Mp 234-236°.

*Amide: 1-Acetyl-9*H*-pyrido[3,4-*b*]indole-3-carboxamide, 9CI.* ***Stellarine A***†
[157341-07-6]
$C_{14}H_{11}N_3O_2$ 253.26
Alkaloid from the roots of *Stellaria dichotoma* var. *lanceolata*.

[2Z-(Methoxycarbonyl)vinyl]amide: ***Stellarine B***†
[180681-40-7]
$C_{18}H_{15}N_3O_4$ 337.334
Alkaloid from the roots of *Stellaria dichotoma* var. *lanceolata*.

[2-(Methoxycarbonyl)ethyl]amide: ***Dichotomide I***
[755036-54-5]
$C_{18}H_{17}N_3O_4$ 339.35
Alkaloid from the roots of *Stellaria dichotoma* var. *lanceolata*. Yellow powder. λ_{max} 220 (log ϵ 3.43); 286 (log ϵ 3.49) (MeOH).

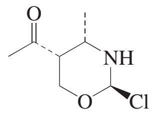
1′S-Alcohol: 1-(1-Hydroxyethyl)-β-carboline-3-carboxylic acid. ***Dichotomine A***

[755036-38-5]
$C_{14}H_{12}N_2O_3$ 256.26
Alkaloid from the roots of *Stellaria dichotoma* var. *lanceolata*. Yellow powder. $[\alpha]_D^{27}$ -9.7 (c, 0.85 in MeOH). λ_{max} 236 (log ϵ 4.14); 269 (log ϵ 4.24) (MeOH).

Faini, F. *et al., Phytochemistry*, 1978, **17**, 338 (*isol, uv, ir, pmr, ms, struct, synth, deriv*)
Razmilić, I. *et al., J. Het. Chem.*, 1980, **17**, 595 (*synth, uv, ir, pmr, ms*)
Faini, F. *et al., Planta Med.*, 1980, **38**, 128 (*isol*)
Cui, Z.-H. *et al., Nat. Prod. Lett.*, 1995, **7**, 59-64 (*Stellarines*)
Sun, B. *et al., J. Nat. Prod.*, 2004, **67**, 1464-1469 (*Dichotomide I, Dichotomine A*)
Omura, K. *et al., Chem. Pharm. Bull.*, 2008, **56**, 237-238 (*Dichotomine A*)

5-Acetyl-2-chlorotetrahydro-4-methyl-2*H*-1,3-oxazine A-46

*1-(2-Chlorotetrahydro-4-methyl-2*H*-1,3-oxazin-5-yl)ethanone*



(2*R**,4*S**,5*R**)*-form*

$C_7H_{12}ClNO_2$ 177.63

(2R*,4S*,5R*)-form [1010693-65-8]
Prod. by *Geotrichum* sp. AL4.
Amorph. solid. $[\alpha]_D^{25}$ +18 (c, 0.09 in $CHCl_3$).

(2R*,4S*,5S*)-form [1010693-64-7]
Prod. by *Geotrichum* sp. AL4.
Amorph. solid. $[\alpha]_D^{25}$ +25 (c, 0.1 in $CHCl_3$).

Li, G.-H. *et al., Chem. Biodiversity*, 2007, **4**, 1520-1524 (*isol, pmr, cmr*)

Acetylcholine(1+) A-47

*2-Acetyloxy-*N,N,N*-trimethylethanaminium, 9CI. Choline acetate*
[51-84-3]
$Me_3N^{\oplus}CH_2CH_2OAc$
$C_7H_{16}NO_2^{\oplus}$ 146.209
Occurs in blood, spleen, ergot and plants and in brain tissue in complexed form e.g. in ergot and *Capsella bursa-pastoris* (shepherd's purse) (Brassicaceae). Neurotransmitter, cholinergic and miotic agent, cardiac depressant, peripheral vasodilator. Easily hyd. by alkalis, and *in vivo* by cholinesterases.

▶ FZ9700000

Chloride: ***Acetylcholine chloride, BAN, INN, USAN****. Miochol. Ovisot*
[60-31-1]
$C_7H_{16}ClNO_2$ 181.662
V. deliquescent cryst. powder. Sol. H_2O. Mp 149-152°.

▶ LD_{50} (rat, orl) 2500 mg/kg. LD_{50} (rat, ivn) 22 mg/kg. FZ9800000

Bromide: [66-23-9]
$C_7H_{16}BrNO_2$ 226.113
Deliquescent prisms (EtOH). Mp 143°.

▶ FZ9680000

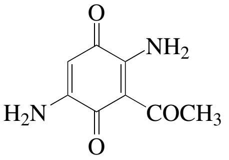
Iodide: [2260-50-6]
$C_7H_{16}INO_2$ 273.113
Mp 161°.

▶ KH3300000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 678C; 678D; 679A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1078A (*nmr*)
Dudley, H.W. *et al., Biochem. J.*, 1929, **23**, 1064 (*synth, bibl*)
Marquardt, P. *et al., Arzneim.-Forsch.*, 1956, **6**, 168; 309 (*biosynth*)
Culvenor, C.C.J. *et al., Chem. Comm.*, 1966, 537 (*pmr*)
Beveridge, D.L. *et al., J.A.C.S.*, 1971, **93**, 3759 (*struct*)
Micelson, M.J. *et al., Acetylcholine; Approach of Mol. Mech. of Action*, Pergamon, 1974,
Hanin, I. *et al., Choline Acetylcholine: Handb. Chem. Assay Methods*, Raven Press, NY, 1974, (*anal*)
Svinning, T. *et al., Acta Cryst. B*, 1975, **31**, 1581 (*cryst struct*)
Sax, M. *et al., Acta Cryst. B*, 1976, **32**, 1953 (*conformn*)
Takasuka, M. *et al., J.C.S. Perkin 2*, 1982, 585 (*ir*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1112
Al-Badr, A.A. *et al., Anal. Profiles Drug Subst.*, 2004, **31**, 3-115 (*chloride, rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABO000; CMF250

3-Acetyl-2,5-diamino-1,4-benzoquinone A-48

[16791-08-5]



$C_8H_8N_2O_3$ 180.163
Constit. of *Cynanchum wilfordii*. Amorph. red powder. Mp > 300°. λ_{max} 304 (log ϵ 4.21); 325 (log ϵ 4.34); 477 (log ϵ 2.87) (DMSO).

N^2,N^5*-Di-Me:* [16791-09-6]
$C_{10}H_{12}N_2O_3$ 208.216
Mp 197°.

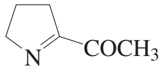
N^5,N^5*-Di-Me:* [16789-18-7]
$C_{10}H_{12}N_2O_3$ 208.216
Mp 164°.

N^2,N^2,N^5,N^5*-Tetra-Me:* [16735-85-6]
$C_{12}H_{16}N_2O_3$ 236.27
Mp 180°.

Schaefer, W. *et al., Tet. Lett.*, 1967, 4307 (*synth*)
Yeo, H. *et al., Phytochemistry*, 1997, **46**, 1103-1105 (*isol, uv, ir, pmr, cmr, ms*)

5-Acetyl-3,4-dihydro-2*H*-pyrrole A-49

*1-(3,4-Dihydro-2*H*-pyrrol-5-yl)ethanone, 9CI. 2-Acetyl-1-pyrroline*
[85213-22-5]

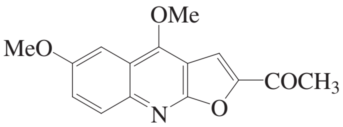


C_6H_9NO 111.143
Isol. from the flowers of *Vallaris glabra*. Key aroma component of rice. Liq. with popcorn odour. Bp_{15} 26-28°. Unstable. Odour threshold of 0.02ng/L in air.

Buttery, R.G. *et al., Chem. Ind. (London)*, 1982, 958; 1983, 478 (*isol, synth*)
Favino, T.F. *et al., J.O.C.*, 1996, **61**, 8975-8979 (*synth, pmr, bibl*)
Hofman, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 616-619; 2270-2277 (***synth, ms, bibl***)
Wongpornchai, S. *et al., J. Agric. Food Chem.*, 2003, **51**, 457-462 (*isol*)
Harrison, T.J. *et al., J.O.C.*, 2005, **70**, 10872-10874 (*synth*)
Adams, A. *et al., Chem. Rev.*, 2006, **106**, 2299-2319 (*rev*)
Snowdon, E.M. *et al., J. Agric. Food Chem.*, 2006, **54**, 6465-6474 (*rev*)
Fuganti, C. *et al., Tetrahedron*, 2007, **63**, 4762-4767 (*synth*)

2-Acetyl-4,6-dimethoxyfuro[2,3-*b*]quinoline A-50

2-Acetylpteleine



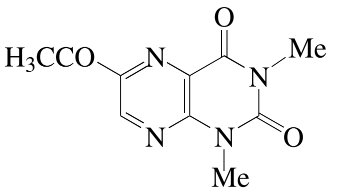
$C_{15}H_{13}NO_4$ 271.272
Alkaloid from the root bark of *Melicope semecarpifolia*. Yellow needles (MeOH). Mp 123-126°. λ_{max} 236 (log ϵ 4.01); 303 (log ϵ 3.7); 330 (log ϵ 3.76) (MeOH).

*6-Demethoxy, 7-methoxy: 2-Acetyl-4,7-dimethoxyfuro[2,3-*b*]quinoline.* ***2-Acetylevolitrine***
$C_{15}H_{13}NO_4$ 271.272
Alkaloid from the root bark of *Melicope semecarpifolia*. Yellow needles (MeOH). Mp 121-124°. λ_{max} 235 (log ϵ 4.41); 260 (log ϵ 4.4); 351 (log ϵ 4.43) (MeOH).

Chen, I.S. *et al., J. Nat. Prod.*, 2001, **64**, 1143-1147

6-Acetyl-1,3-dimethyl-2,4(1*H*,3*H*)-pteridinedione, 9CI A-51

6-Acetyl-1,3-dimethyllumazine
[94591-18-1]

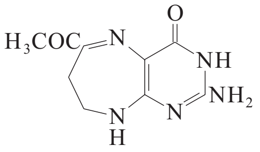


$C_{10}H_{10}N_4O_3$ 234.214
Isol. from the marine polychaete worm *Odontosyllis undecimdonta*. Needles (MeOH). Mp 177-178° (173°).

Kakoi, H. *et al., Heterocycles*, 1995, **41**, 789-797 (*isol, synth, pmr, cmr*)

6-Acetylhomopterin A-52

*6-Acetyl-2-amino-1,7,8,9-tetrahydro-4*H*-pyrimido[4,5-*b*][1,4]diazepin-4-one, 9CI. Quench spot*
[80003-63-0]

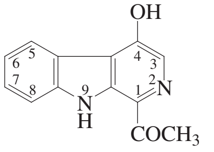


$C_9H_{11}N_5O_2$ 221.218
Naturally occurring diazepine from *Drosophila melanogaster*. Intermed. involved in the biosynth. of Drosopterin, D-941. Greenish-yellow cryst.

Wiederrecht, G.J. *et al., J. Biol. Chem.*, 1981, **256**, 10399 (*isol, struct, ms, pmr*)
Jacobson, K.B. *et al., Biochemistry*, 1982, **21**, 5700 (*isol, struct, pmr, cmr, uv*)
Boyle, P.H. *et al., Tet. Lett.*, 1987, **28**, 5331 (*synth*)

1-Acetyl-4-hydroxy-β-carboline A-53

*1-(4-Hydroxy-9*H*-pyrido[3,4-*b*]indol-1-yl)ethanone, 9CI*



$C_{13}H_{10}N_2O_2$ 226.234

Me ether: ***1-Acetyl-4-methoxy-β-carboline***
[65236-63-7]
$C_{14}H_{12}N_2O_2$ 240.261
Alkaloid from the bark and roots of *Ailanthus malabarica* and from the root bark of *Ailanthus altissima* (Simaroubaceae). Prisms. Mp 208° 204-205° Mp 212.5-214°. λ_{max} 238 (log ϵ 4.15); 270 (log ϵ 4.26); 288 (log ϵ 4.23); 370 (log ϵ 3.82) (EtOH).

Joshi, B.S. *et al., Heterocycles*, 1977, **7**, 193-200 (*isol, uv, ir, pmr, ms, struct*)
Ohmoto, T. *et al., Chem. Pharm. Bull.*, 1981, **29**, 390-395 (*isol, uv, ir, pmr, cmr, ms*)
Koike, K. *et al., Org. Magn. Reson.*, 1984, **22**, 471-473 (*cmr*)
Suzuki, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2170-2172 (*synth*)
Suzuki, H. *et al., Tetrahedron*, 1997, **53**, 1593-1606 (*synth*)

1-Acetyl-6-hydroxy-β-carboline A-54

*1-(6-Hydroxy-9*H*-pyrido[3,4-*b*]indol-1-yl)ethanone, 9CI*
$C_{13}H_{10}N_2O_2$ 226.234

O-*(4-*O*-Methyl-β-*D*-glucopyranoside):* ***BB 4***
$C_{20}H_{22}N_2O_7$ 402.403
Isol. from the oriental crude drug bombyx batryticatus (dried larvae of *Bombyx mori*).

Kikuchi, H. *et al., Tet. Lett.*, 2004, **45**, 367-370 (*BB4*)

1-Acetyl-7-hydroxy-β-carboline A-55

*1-(7-Hydroxy-9*H*-pyrido[3,4-*b*]indol-1-yl)ethanone, 9CI.* ***Arenarine D***
[123520-96-7]

$C_{13}H_{10}N_2O_2$ 226.234
Alkaloid from *Arenaria kansuensis* (Caryophyllaceae). Pale yellow needles (EtOAc). Mp 176-177° dec.

O-*(4-*O*-Methyl-β-*D*-glucopyranoside):* ***BB 3***
$C_{20}H_{22}N_2O_7$ 402.403
Isol. from the oriental crude drug, bombyx batryticatus (dried silkworms, *Bombyx* spp.).

Me ether: 1-Acetyl-7-methoxy-β-carboline. ***Arenarine C***
[62230-10-8]
$C_{14}H_{12}N_2O_2$ 240.261
Alkaloid from *Banisteriopsis caapi* (Malphigiaceae) and from the whole plant of *Arenaria kansuensis* (Caryophyllaceae). Light yellow needles ($CHCl_3$ or hexane/EtOAc). Mp 224-225° dec. (190° dec.). λ_{max} 260 (log ϵ 4.18); 289 (log ϵ 4.37); 334 (log ϵ 4.02) ($CHCl_3$).

Hashimoto, Y. *et al., Phytochemistry*, 1976, **15**, 1559-1560 (*Me ether, isol, synth, pmr*)
Wu, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1808 (*isol, uv, ir, pmr, cmr, ms*)
Kikuchi, H. *et al., Tet. Lett.*, 2004, **45**, 367-370 (*BB 3*)

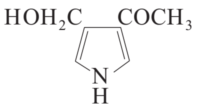
1-Acetyl-8-hydroxy-β-carboline A-56

*1-(8-Hydroxy-9*H*-pyrido[3,4-*b*]indol-1-yl)ethanone, 9CI*
$C_{13}H_{10}N_2O_2$ 226.234
Alkaloid from *Hypodematium squamuloso-pilosum*. Pale yellow powder (MeOH aq.). Mp 242-243°. λ_{max} 256 ; 277 ; 310 ; 390 (MeOH).

Zhou, T.-S. *et al., Phytochemistry*, 1998, **49**, 1807-1809 (*isol, uv, ir, pmr, cmr, ms*)

3-Acetyl-4-(hydroxymethyl)-pyrrole A-57

*1-[4-(Hydroxymethyl)-1*H*-pyrrol-3-yl]ethanone, 9CI.* ***Verrucarin E***
[24445-13-4]

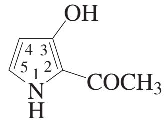


$C_7H_9NO_2$ 139.154
Pyrrole antibiotic. Metab. of *Myrothecium verrucaria*. Shows cytostatic activity. Cryst. (Et_2O/Me_2CO). Sol. EtOAc; poorly sol. H_2O, acids, bases. Mp 90.5-91°. λ_{max} 260 (ϵ 17800) (MeOH or EtOH) (Derep). λ_{max} 249 (ϵ 10000) (EtOH) (Berdy).
Ac:
$C_9H_{11}NO_3$ 181.191
Cryst. (Et_2O/Me_2CO). Mp 102°.

Härri, E. *et al., Helv. Chim. Acta*, 1962, **45**, 839 (*isol, props*)
Pfäffli, P. *et al., Helv. Chim. Acta*, 1969, **52**, 1911-1920; 1921-1929 (*struct, biosynth*)
Gossauer, A. *et al., Helv. Chim. Acta*, 1976, **59**, 1698-1704 (*synth*)
Sheldrick, W.S. *et al., Acta Cryst. B*, 1978, **34**, 1248-1253 (*cryst struct*)
Chexal, K.K. *et al., Helv. Chim. Acta*, 1980, **63**, 761 (*biosynth*)
Muchowski, J.M. *et al., Helv. Chim. Acta*, 1984, **67**, 1168 (*synth*)
Adinolfi, A. *et al., J. Agric. Food Chem.*, 2005, **53**, 1598-1603 (*isol, cmr, ms*)

2-Acetyl-3-hydroxy-1*H*-pyrrole A-58

*1-(3-Hydroxy-1*H*-pyrrol-2-yl)ethanone*
[95232-59-0]



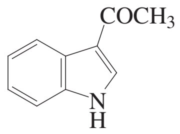
$C_6H_7NO_2$ 125.127

O-*[β-*D*-Fucopyranosyl-(1→3)-β-*D*-fucopyranosyl-(1→4)-[6-deoxy-β-*D*-glucopyranosyl-(1→2)]-6-deoxy-β-*D*-glucopyranoside]:*
$C_{30}H_{47}NO_{18}$ 709.697
Alkaloid from the starfish *Asterina pectinifera*. Amorph. powder. Mp 240-245°. $[\alpha]_D^{18}$ +0.2 (c, 0.3 in MeOH).
*Me ether: 2-Acetyl-3-methoxy-1*H*-pyrrole*
[70718-05-7]
$C_7H_9NO_2$ 139.154
Needles (H_2O). Mp 115-116°.

Fisher, B.E. *et al., J.O.C.*, 1964, **29**, 776-781 (*Me ether*)
Zhang, L.-X. *et al., Nat. Prod. Res.*, 2006, **20**, 229-233 (*isol, pmr, cmr, ms*)

3-Acetylindole A-59

*1-(1*H*-Indol-3-yl)ethanone, 9CI. 3-Indolyl methyl ketone*
[703-80-0]

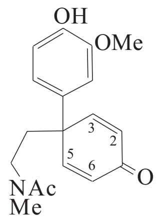


$C_{10}H_9NO$ 159.187
Constit. of *Strychnos cathayensis*. Cryst. (cyclohexane/EtOH). Spar. sol. H_2O. Mp 194°. pK_a 12.99 (25°,NH).
▶ LD_{50} (mus, ipr) 300 mg/kg. OB4520000
Picrate:
Yellow cryst. (petrol). Mp 183°.
Oxime: [87052-79-7]
[40747-12-4 (*E*-form), 40747-13-5 (*Z*-form)]
$C_{10}H_{10}N_2O$ 174.202
Mp 144-147°. Oximation produces the *E*-form.
N-*Ac:* [17537-64-3]
$C_{12}H_{11}NO_2$ 201.224
Sol. hot H_2O. Mp 151°. Sublimes.
N-*Me: 3-Acetyl-1-methylindole*
[19012-02-3]
$C_{11}H_{11}NO$ 173.214
Cryst. (EtOH). Mp 104-105°. $Bp_{0.01}$ 130-140°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 666A (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 135C (*nmr*)
Baker, J.W. *et al., J.C.S.*, 1946, 461-463 (*synth, N-Ac*)
Pyang, H.-S. *et al., Chem. Comm.*, 1972, 77 (*synth*)
Rosenberg, E. *et al., Org. Magn. Reson.*, 1976, **8**, 117 (*nmr*)
Pindur, U. *et al., Annalen*, 1986, 1621 (*synth, ir, pmr*)
Kasahara, A. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 927 (*synth*)
Majchrzak, M.W. *et al., Synthesis*, 1986, 956-958 (*N-Me, synth, pmr*)
Shner, V.F. *et al., Chem. Heterocycl. Compd. (Engl. Transl.)*, 1989, 272-274 (*N-Ac, synth*)
Bergman, J. *et al., Tetrahedron*, 1990, **46**, 6061 (*synth*)
Pindur, U. *et al., Helv. Chim. Acta*, 1991, **74**, 727-738 (*E-form, oxime, synth, pmr, ms*)
Yang, C.X. *et al., Synth. Commun.*, 1997, **27**, 2125-2132 (*synth, pmr, cmr, ms*)
Cheng, M.-J. *et al., J. Chin. Chem. Soc. (Taipei)*, 2001, **48**, 235-239 (*isol*)
Taira, S. *et al., Tet. Lett.*, 2002, **43**, 8893-8896 (*N-Ac, synth, pmr*)
Wynne, J.H. *et al., Synthesis*, 2004, 2277-2282 (*synth, ir, pmr, cmr*)

4-[2-(Acetylmethylamino)-ethyl]-4-(4-hydroxy-3-methoxy-phenyl)-2,4-cyclohexadien-1-one **A-60**
N-*Methyl-4′*-O-*demethyl*-N,7a-*secomesembradienone*
[82545-13-9]



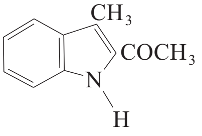
$C_{18}H_{21}NO_4$ 315.368

Achiral molecule. Alkaloid from *Sceletium namaquense* (Aïzoaceae). Mp 107.5°.

2,3,5,6-Tetrahydro, Me ether: ***4-[2-(Acetylmethylamino)ethyl]-4-(3,4-dimethoxyphenyl)cyclohexanone***. N-*Acetyl*-N-*methyl*-N,7a-*secomesembrine*
[82545-07-1]
$C_{19}H_{27}NO_4$ 333.427
Alkaloid from *Sceletium namaquense* (Aïzoaceae). Oil.

Jeffs, P.W. *et al., J.O.C.*, 1982, **47**, 3611 (*isol, ir, pmr, ms, struct, synth*)

2-Acetyl-3-methylindole **A-61**
*1-(3-Methyl-1*H*-indol-2-yl)ethanone, 9CI.* ***Salvadoricine***
[16244-23-8]

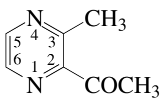


$C_{11}H_{11}NO$ 173.214

The first naturally occurring 2-acetylindole alkaloid. Alkaloid from the leaves of *Salvadora persica* (Salvadoraceae). Needles (hexane). Mp 146-147° (143-144°).

Ishizumi, K. *et al., Chem. Pharm. Bull.*, 1967, **15**, 863 (*synth*)
Jackson, A.H. *et al., Chem. Comm.*, 1978, 779 (*synth*)
Malik, S. *et al., Tet. Lett.*, 1987, **28**, 163 (*isol, uv, ir, pmr, cmr, ms*)
Pindur, U. *et al., J. Het. Chem.*, 1992, **29**, 145 (*synth, pmr, cmr, ms*)

2-Acetyl-3-methylpyrazine **A-62**
1-(3-Methylpyrazinyl)ethanone, 9CI. Methyl (3-methylpyrazinyl) ketone, 8CI
[23787-80-6]

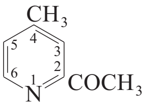


$C_7H_8N_2O$ 136.153

Present in spiny lobster *Panulirus argus*. Liq. with burnt, popcorn-like odour. d 1.11. Bp$_{0.5}$ 56°. n_D^{20} 1.5216. Odour threshold 2 x 10^{-2} ppm in H_2O.

Mookherjee, B.D. *et al., J.O.C.*, 1972, **37**, 511-513 (*synth, ir, pmr, ms*)
Wolt, J. *et al., J.O.C.*, 1975, **40**, 1178-1179 (*synth, pmr, ms*)
Mihara, S. *et al., J. Agric. Food Chem.*, 1988, **36**, 1242-1247 (*props*)
Nakamura, S. *et al., Agric. Biol. Chem.*, 1989, **53**, 1891-1899 (*glc, occur*)
Cadwallader, K.R. *et al., J. Agric. Food Chem.*, 1995, **43**, 2432-2437 (*detn, occur*)

2-Acetyl-4-methylpyridine **A-63**
1-(4-Methyl-2-pyridinyl)ethanone, 9CI. Methyl 4-methyl-2-pyridyl ketone, 8CI. 2-Acetyl-4-picoline
[59576-26-0]



C_8H_9NO 135.165

Component of tobacco smoke and fig leaf absolute (*Ficus carica*). Cryst. (petrol). Sol. EtOH. Mp 33-34°. Bp$_{15}$ 95-97°.

*Oxime (*E-*):* [23089-35-2]
$C_8H_{10}N_2O$ 150.18
Used as a 0.01*M* soln. in EtOH for photometric detn. of Co (λ_{max} 325 nm, ϵ 11800, EtOH aq.), Cu(*I*) (λ_{max} 409 nm, ϵ 5300, EtOH aq.), extraction-photometric detn. of Fe(*II*) (λ_{max} 541 nm, ϵ 14000, isopentanol). Cryst. (C_6H_6/petrol). Mp 98-99° Mp 125-128°.

Semicarbazone:
Solid. Mp 195-198°.

[18103-84-9]

Case, F.H. *et al., J.A.C.S.*, 1956, **78**, 5842 (*synth*)
Nishimoto, N. *et al., Yakugaku Zasshi*, 1961, **81**, 88; *CA*, **55**, 13421b (*synth*)
Case, F.H. *et al., J. Het. Chem.*, 1968, **5**, 161 (*synth, oxime*)
Schilt, A. *et al., Talanta*, 1969, **16**, 448 (*detn, Co, Cu, Fe*)

2-Acetyl-6-methylpyridine **A-64**
1-(6-Methyl-2-pyridinyl)ethanone, 9CI. Methyl 6-methyl-2-pyridyl ketone, 8CI. 6-Acetyl-2-picoline
[6940-57-4]

C_8H_9NO 135.165

Minor component of rum and tobacco smoke. Flavour modifying agent for coffee. Liq. Bp$_1$ 46°.

*Oxime (*E-*):* [23089-39-6]
$C_8H_{10}N_2O$ 150.18
Used as a 0.01*M* soln. in EtOH for photometric detn. of Cu(*I*) (λ_{max} 422 nm, ϵ 8400, EtOH aq.). Cryst. (petrol). Sol. EtOH. Mp 49-50°.

Dimethylhydrazone: [33785-80-7]
$C_{10}H_{15}N_3O$ 193.248
Liq. Bp$_{0.1}$ 53-54°. n_D^{26} 1.5370.

[18103-88-3]

Case, F.H. *et al., J. Het. Chem.*, 1968, **5**, 161 (*synth, oxime*)
Schilt, A. *et al., Talanta*, 1969, **16**, 448 (*detn, Cu*)
Newkome, G.R. *et al., J.O.C.*, 1972, **37**, 1329 (*deriv*)
Zanger, M. *et al., Anal. Chem.*, 1974, **46**, 2042 (*pmr*)
Amin, H.B. *et al., J.C.S. Perkin 2*, 1979, 624 (*synth*)

3-Acetyl-2-methylpyridine **A-65**
1-(2-Methyl-3-pyridinyl)ethanone, 9CI. Methyl 2-methyl-3-pyridyl ketone, 8CI. 3-Acetyl-2-picoline
[1721-12-6]

C_8H_9NO 135.165

Pheromone present in ferret (*Mustela putorius*) urine. Prisms. Mp 30-31°. Bp$_{15}$ 99-100°.

Dipicrate:
Needles (EtOH). Mp 174-176°.

Baumgarten, P. *et al., Ber., B*, 1939, **72**, 563 (*synth*)
Sanders, E.B. *et al., J.O.C.*, 1978, **43**, 324 (*synth, pmr, ir*)

3-Acetyl-4-methylpyridine **A-66**
1-(4-Methyl-3-pyridinyl)ethanone, 9CI. Methyl 4-methyl-3-pyridyl ketone, 8CI. 3-Acetyl-4-picoline
[51227-30-6]

C_8H_9NO 135.165

Pheromone from ferret (*Mustela putorius*) urine. Volatile liq. Bp$_{1.5}$ 57-58° (lit. gives a pressure range).

Picrate:
Solid (EtOH). Mp 146-147°.

Webb, J.L. *et al., J.A.C.S.*, 1944, **66**, 1456 (*synth*)
Deuchert, K. *et al., Chem. Ber.*, 1979, **112**, 2045 (*synth, pmr*)
Rey, A.W. *et al., Can. J. Chem.*, 1992, **70**, 2922 (*synth, ir, pmr, cmr, ms*)

4-Acetyl-2-methylpyridine **A-67**
1-(2-Methyl-4-pyridinyl)ethanone, 9CI. Methyl 2-methyl-4-pyridyl ketone, 8CI. 4-Acetyl-2-picoline
[2732-28-7]

C_8H_9NO 135.165

Component of roasting coffee aroma. Pheromone present in ferret (*Mustela putorius*) urine. Liq. Bp$_{10}$ 120-124° Bp$_4$ 130°.

Picrate: [31931-61-0]
Solid (EtOH). Mp 174-175°.

[80882-67-3]

Suzuki, Y. *et al., Yakugaku Zasshi*, 1961, **81**, 795; *CA*, **55**, 24742d (*synth*)
Eilhauer, H.D. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1965, **298**, 131 (*synth*)
Govindachari, T.R. *et al., Indian J. Chem.*, 1966, **4**, 398 (*synth*)

4-Acetyl-3-methylpyridine A-68

1-(3-Methyl-4-pyridinyl)ethanone, 9CI. Methyl 3-methyl-4-pyridyl ketone, 8CI. 4-Acetyl-3-picoline
[82352-00-9]

C_8H_9NO 135.165
Pheromone from ferret (*Mustela putorius*) urine. Bp_1 93-95°.

Hibino, S. *et al., J. Het. Chem.*, 1990, **27**, 1751 (*synth, pmr, ms*)

5-Acetyl-2-methylpyridine A-69

1-(6-Methyl-3-pyridinyl)ethanone, 9CI. Methyl 6-methyl-3-pyridyl ketone, 8CI. 5-Acetyl-2-picoline
[36357-38-7]

C_8H_9NO 135.165
Minor component of palmarosa oil and tobacco smoke. Used in perfume compositions. Liq. Bp_{15} 105-106°.

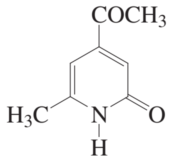
2,4-Dinitrophenylhydrazone: [40624-50-8]
Solid. Mp 224-225°.

[65305-38-6]

Muruoka, M. *et al., Nippon Kagaku Zasshi*, 1961, **82**, 1279; *CA*, **59**, 563b (*synth*)
Hawkins, E.G.E. *et al., J.C.S. Perkin 1*, 1972, 2882 (*synth*)
Kozerski, L. *et al., Org. Magn. Reson.*, 1977, **9**, 395 (*cmr*)
Markova, N.K. *et al., Zh. Org. Khim.*, 1984, **20**, 962 (*synth*)

4-Acetyl-6-methyl-2(1*H*)-pyridinone A-70

4-Acetyl-2-hydroxy-6-methylpyridine. ***Streptokordin***

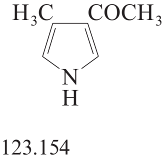


$C_8H_9NO_2$ 151.165
Prod. by a marine-derived *Streptomyces* sp. KORDI-3238. Cytotoxic. Amorph. powder. λ_{max} 217 (ϵ 10500) (MeOH).

Jeong, S.-Y. *et al., J. Antibiot.*, 2006, **59**, 234-240 (*isol, pmr, cmr*)

3-Acetyl-4-methylpyrrole A-71

*1-(4-Methyl-1*H*-pyrrol-3-yl)ethanone, 9CI.* ***Deoxyverrucarin E***
[18818-30-9]



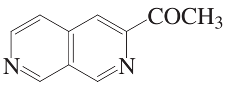
C_7H_9NO 123.154
Pyrrole antibiotic. Metab. of *Eupenicillium hirayamae*. Possesses antitumour activity. Cryst. (C_6H_6/hexane). Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. Mp 115°. λ_{max} 247 (ϵ 11070); 277 (ϵ 2204) (EtOH) (Berdy).

Semicarbazone:
Pale-yellow needles (MeOH). Mp 195°.

V. Leusen, A.M. *et al., Tet. Lett.*, 1972, 5337 (*pmr*)
Arndt, R.R. *et al., Phytochemistry*, 1974, **13**, 1865-1870 (*isol, struct*)
Cheng, D.O. *et al., Tet. Lett.*, 1977, 1469 (*synth*)
Arai, K. *et al., Chem. Pharm. Bull.*, 1983, **31**, 925 (*synth, uv, ir, pmr*)

3-Acetyl-2,7-naphthyridine A-72

1-(2,7-Naphthyridin-3-yl)ethanone, 9CI
[73607-00-8]

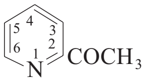


$C_{10}H_8N_2O$ 172.186
Alkaloid from valerian (*Valeriana officinalis*).

Janot, M.M. *et al., Ann. Pharm. Fr.*, 1979, **37**, 413-420 (*isol, cryst struct*)
Barbu, E. *et al., Heterocycl. Commun.*, 2000, **6**, 25-28 (*synth*)

2-Acetylpyridine A-73

1-(2-Pyridinyl)ethanone, 9CI. Methyl 2-pyridyl ketone. 2-Acetopyridine. FEMA 3251
[1122-62-9]



C_7H_7NO 121.138
Present in various cooked and treated food. Present in coriander seed and black tea. Organoleptic, flavouring agent. Liq. with roasted odour. Bp 192°. n_D^{20} 1.5203. pK_a 2.64 (25°). Turns yellow in air.

Hydrochloride: Mp 183-185° dec.

Methiodide: Mp 161°.

Ethiodide: Mp 205°.

Picrate:
Yellow cryst. (EtOH). Mp 131°.

Oxime: Acepox
[1758-54-9]
$C_7H_8N_2O$ 136.153
Plant protectant. Used for photometric detn. of Re (λ_{max} 490 nm, ϵ 3800). Prisms (EtOH). Sol. H_2O. Mp 121°.

Hydrazone: [59742-91-5]
$C_7H_9N_3$ 135.168
Used as 0.5m*M* aq. soln. for fluorimetric detn. of Tc(*VII*) (λ_{max} 430 nm, 0.01-10μg/ml, =1.4*M* HCl). Cryst. (EtOH). Sol. H_2O, EtOH.

Phenylhydrazone: [7734-05-6]
Yellow cryst. (EtOH). Mp 155°.

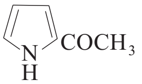
Thiosemicarbazone: [6839-90-3]
$C_8H_{10}N_4S$ 194.26
Used as EtOH soln. or 1% Me_2CO aq. soln. for photometric detn. of Mo (λ_{max} 470 nm, ϵ 17000), V (λ_{max} 400 nm, ϵ 56000, pH 3.5). Cryst. (EtOH). Sol. EtOH, DMF, Me_2CO.

Ethylene ketal:
$C_9H_{11}NO_2$ 165.191
$Bp_{0.8}$ 91-95°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 779A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 310A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1542B (*ir*)
Thompson, R.J. *et al., Anal. Chim. Acta*, 1964, **31**, 590 (*oxime, detn, Re*)
Miyajama, G. *et al., Chem. Pharm. Bull.*, 1972, **20**, 429 (*cmr*)
Lesman, T. *et al., Org. Mass Spectrom.*, 1973, **7**, 1321 (*ms*)
Seth-Paul, W.A. *et al., Spectrochim. Acta A*, 1974, **30**, 1817 (*ir*)
Reimann, E. *et al., Annalen*, 1976, 1351 (*synth*)
Klayman, D.L. *et al., J. Med. Chem.*, 1979, **22**, 855 (*synth, thiosemicarbazone*)
Grases, F. *et al., Anal. Chim. Acta*, 1984, **166**, 71 (*synth, detn, Tc*)
Thimmaiah, K.N. *et al., Microchem. J.*, 1985, **32**, 8 (*detn, Mo*)
Norman, M.H. *et al., J.O.C.*, 1987, **52**, 226 (*deriv, synth, ir, pmr, cmr*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 35 (*occur*)
Girardot, M. *et al., J.O.C.*, 1998, **63**, 10063-10068 (*synth*)

2-Acetylpyrrole A-74

*1-(1*H*-Pyrrol-2-yl)ethanone, 9CI. Methyl 2-pyrrolyl ketone. 2-Acetopyrrole. Pseudoacetylpyrrole. FEMA 3202*
[1072-83-9]



C_6H_7NO 109.127
Found in *Valeriana officinalis* (Valerianaceae), *Camellia sinensis* (Theaceae), *Paeonia moutan* (Chinese drug Botanpi) (Peoniaceae), *Lycium chinense* (Solanaceae). Prod. by *Streptomyces* sp. A-5071. Organoleptic which contributes to many aromas, including tobacco smoke. Flavouring agent. Possesses hepatoprotective props. Cryst. (petrol) with bread-like odour. Sol. H_2O. Mp 90°. Bp 220°. λ_{max} 247 ; 287 (MeOH) (Berdy).

Oxime: [63547-59-1]
$C_6H_8N_2O$ 124.142
Mp 145-146°.

Phenylhydrazone: Mp 146°.

2,4-Dinitrophenylhydrazone:
Reddish-brown cryst. Mp 297° dec.

Semicarbazone: Mp 190°.

N-*(4-Methylbenzenesulfonyl):* [129666-99-5]
$C_{13}H_{13}NO_3S$ 263.317
Solid ($CHCl_3$/hexane). Mp 110-111°.

N-*Me: 2-Acetyl-1-methylpyrrole. FEMA 3184*

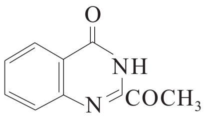
[932-16-1]
C_7H_9NO 123.154
Bp 200-202°. n_D^{20} 1.5420.

N-*Et: 2-Acetyl-1-ethylpyrrole. FEMA 3147*
[39741-41-8]
$C_8H_{11}NO$ 137.181
Bp_{12} 82°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 567D; 568A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 5B; 5C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1447B; 1447C (*ir*)
Cionga, E. *et al., C. R. Hebd. Seances Acad. Sci.*, 1935, **200**, 780 (*isol*)
Sugisawa, H. *et al., Chem. Ind. (London)*, 1958, 887 (*synth*)
Budzikiewicz, H. *et al., J.C.S.*, 1964, 1949 (*ms*)
Abraham, R.J. *et al., J.C.S. Perkin 2*, 1974, 1004 (*cmr*)
Sannai, A. *et al., Agric. Biol. Chem.*, 1983, **47**, 2397 (*isol*)
Miyayawa, M. *et al., Agric. Biol. Chem.*, 1983, **47**, 2925; 1984, **48**, 2847 (*isol*)
Kakushima, M. *et al., J.O.C.*, 1983, **48**, 3214 (*synth*)
Garrido, D.O.A. *et al., J.O.C.*, 1984, **49**, 2619 (*synth*)
Anderson, H.J. *et al., Can. J. Chem.*, 1985, **63**, 896 (*synth*)
Eyley, S.C. *et al., Tet. Lett.*, 1985, **26**, 4649 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ADA 375
Pindur, H. *et al., J. Het. Chem.*, 1989, **26**, 1563 (*ir*)
Kuroda, Y. *et al., Tet. Lett.*, 1989, **30**, 2411 (*synth*)
Ito, M. *et al., Agric. Biol. Chem.*, 1991, **55**, 2117 (*isol, props*)
Goldberg, Yu. *et al., Synth. Commun.*, 1991, **21**, 557 (*N-alkyl derivs, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 215; 468; 560
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 944; 1709; 1853-1854 (*occur, props, use*)
Hou, S. *et al., Macromolecules*, 2003, **36**, 3826-3832 (*synth, N-tosyl*)
Camarillo, C.A. *et al., Acta Cryst. E*, 2007, **63**, o2593-o2594 (*cryst struct*)

2-Acetyl-4(3*H*)-quinazolinone A-75

[17244-28-9]

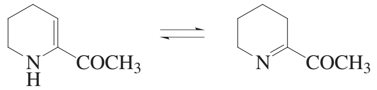


$C_{10}H_8N_2O_2$ 188.185
Fungal metab. prod. from a toxic strain of *Fusarium culmorum*. Also isol. from cultures of *Fusarium sambucinum*. Prisms (EtOAc or Me_2CO). Mp 197-200° dec Mp 205°. Has also been descr. as a transformation prod. of 2-(1-Hydroxyethyl)-4(3*H*)-quinazolinone, H-499, and of 2-Pyruvoylaminobenzamide, from *P. chrysogenum, P. notatum* and *Colletotrichum lagenarium*. Although isol. from the *P. chrysogenum* fermentation, it was considered in that instance to be an artifact. λ_{max} 302 (ε 11600) (MeOH) (Berdy). λ_{max} 232 (H_2O) (Berdy).

Suter, P.J. *et al., J.C.S.(C)*, 1967, 2240 (*synth*)
Blight, M.M. *et al., J.C.S. Perkin 1*, 1974, 1691 (*isol, uv, ir, pmr*)
Niederer, D. *et al., Tet. Lett.*, 1992, **33**, 3997 (*isol*)

6-Acetyl-1,2,3,4-tetrahydropyridine A-76

Methyl 3,4,5,6-tetrahydro-2-pyridyl ketone, 8CI. 2-Acetyl-3,4,5,6-tetrahydropyridine. 2-Acetyl-Δ¹-piperideine. 2-Acetyl-Δ²-piperideine. 1-(1,4,5,6-Tetrahydro-2-pyridinyl)ethanone, 9CI
[27300-27-2]



1*H-form* 3*H-form*

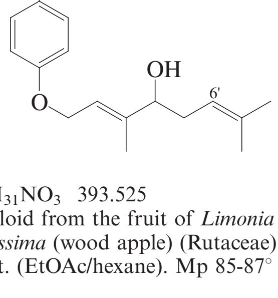
$C_7H_{11}NO$ 125.17
Tautomeric, 1*H*-form predominates *ca.* 2:1. Constit. of the leaves of *Semnostachya menglaensis* (preferred genus name *Strobilanthes*). Key aroma component of bread. Responsible for mousy taint in wines. Unstable liq. Bp_3 65-67°. Odour threshold 0.06 ng/L in air.

Hydrochloride: Mp 112-119°.

Hunter, I.R. *et al., Cereal Chem.*, 1969, **46**, 189 (*isol*)
Büchi, G. *et al., J.O.C.*, 1971, **36**, 609 (*ir, uv, pmr, ms, synth*)
Strauss, C.R. *et al., Chem. Ind. (London)*, 1984, 109 (*isol*)
De Kimpe, N. *et al., J.O.C.*, 1993, **58**, 2904 (*synth, pmr, cmr, ms*)
De Kimpe, N. *et al., Tetrahedron*, 1995, **51**, 2387 (*synth*)
Hofman, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 616-619; 2270-2277 (*synth, ms, bibl*)
Naef, R. *et al., J. Agric. Food Chem.*, 2005, **53**, 9161-9164 (*isol, pmr, ms*)
Harrison, T.J. *et al., J.O.C.*, 2005, **70**, 10872-10874 (*synth*)
Adams, A. *et al., Chem. Rev.*, 2006, **106**, 2299-2319 (*rev*)
Snowdon, E.M. *et al., J. Agric. Food Chem.*, 2006, **54**, 6465-6474 (*rev*)
Fuganti, C. *et al., Tetrahedron*, 2007, **63**, 4762-4767 (*synth*)

Acidissiminol A-77

[126006-00-6]



$C_{25}H_{31}NO_3$ 393.525
Alkaloid from the fruit of *Limonia acidissima* (wood apple) (Rutaceae). Cryst. (EtOAc/hexane). Mp 85-87° .

O-*Ac:* **N-*Benzoyl-4-(4-acetoxyneryloxy)-phenethylamine***
[33055-26-4]
$C_{27}H_{33}NO_4$ 435.562
Alkaloid from fruit of *Swinglea glutinosa* (Rutaceae). Cryst. (EtOAc/hexane). V. sol. MeOH. Mp 64-65°. Opt. inactive. Related to Severine.

O-*Octadecanoyl:* ***Acidissiminin***
[126005-91-2]
$C_{43}H_{65}NO_4$ 659.991
Alkaloid from the fruits of *Limonia acidissima* (wood apple) (Rutaceae). Amorph. solid (EtOAc/hexane). Mp 65°. $[\alpha]_D$ 0 ($CHCl_3$). λ_{max} 225; 277 (sh); 286 (MeOH) (Derep).

6′,7′-Epoxide: ***Acidissiminol epoxide****. Severine*†
[139165-01-8]
[33055-25-3]
$C_{25}H_{31}NO_4$ 409.524
Alkaloid from fruits of *Limonia acidissima* (wood apple) (Rutaceae). Cryst. (MeOH). Mp 146-149° (141-143°). Severine originally considered to be a diol with formula $C_{25}H_{33}NO_4$. Identity of Acidissiminol epoxide and Severine not confirmed; stereochem. not established.

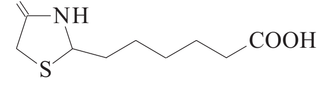
6′,7′-Epoxide, octadecanoyl: ***Acidissiminin epoxide****. Severine palmitate*
[139083-09-3]
$C_{43}H_{65}NO_5$ 675.99
Alkaloid from the fruit of *Limonia acidissima* (wood apple), leaves of *Severinia buxifolia* and from *Pamburus missionis*, *Atalantia monophylla* and *Hesperethusa crenulata* (preferred genus name *Naringi*) (Rutaceae). Cryst. (C_6H_6/hexane). Mp 105-106° Mp 113-114°. Identity of Acidissiminin epoxide and Severin palmitate not definitely establ. Mps are similar.

6′,7′-Dihydro, 6′,7′-dihydroxy: ***Dihydroxyacidissiminol***
[160387-10-0]
$C_{25}H_{33}NO_5$ 427.539
Alkaloid from fruits of *Limonia acidissima* (wood apple) (Rutaceae). Amorph. semi-solid.

Dreyer, D.L. *et al., Tetrahedron*, 1967, **23**, 4613; 1970, **26**, 5745; 1980, **36**, 827 (*Severine, Severine palmitate, N-Benzoyl-4-(4-acetoxyneryloxy)phenethylamine*)
Ghosh, P. *et al., J. Nat. Prod.*, 1989, **52**, 1323; 1991, **54**, 1389 (*Acidissiminol, Acidissiminin*)
Ghosh, P. *et al., Phytochemistry*, 1994, **37**, 757 (*Dihydroxyacidissiminol, Acidissiminol epoxide*)

Acidomycin A-78

4-Oxo-2-thiazolidinehexanoic acid, 9CI. 2-(5-Carboxypentyl)-4-thiazolidone, 8CI. Actithiazic acid. Cinnamonin. Mycobacidin. Thiazolidomycin. PA 95. Antibiotic 6604-4. Antibiotic PA 95
[539-35-5]



$C_9H_{15}NO_3S$ 217.288

Amino acid derived antibiotic. Abs. config. not known. Log P 0.86 (calc).

▶ LD_{50} (mus, ipr) 2500 mg/kg. XJ6000000

(-)-form [28223-69-0]

Prod. by *Streptomyces* spp. Active against mycobacteria *in vitro*. Needles (H_2O, MeOH or Me_2CO). Sol. MeOH, $CHCl_3$, bases; fairly sol. CH_2Cl_2; poorly sol. H_2O, acids, hexane, C_6H_6. Mp 139-140°. $[\alpha]_D^{23}$ -54 (MeOH). $[\alpha]_D^{25}$ -60 (c, 1 in EtOH). Blue fluor. in uv light. Racemised by dil. alkalis. λ_{max} 245 (MeOH) (Berdy).

▶ LD_{50} (mus, ivn) 1500 mg/kg, LD_{50} (mus, ipr) 2500 mg/kg, LD_{50} (mus, scu) 20000 mg/kg.

Me ester:

Needles. Mp 53-54°. $[\alpha]_D^{25}$ -50.9 (MeOH).

(±)-form [106448-99-1]

Needles (H_2O or $CHCl_3$). Mp 122-123° (116-117°).

McLamore, W.M. *et al., J.A.C.S.*, 1952, **74**, 2946-2947 (*struct*)

Sobin, B.A. *et al., J.A.C.S.*, 1952, **74**, 2947-2948 (*isol*)

Miyake, A. *et al., Pharm. Bull.*, 1953, **1**, 84-88 (*isol, struct*)

Japan. Pat., 1954, (*(Takeda)*)54 448; *CA*, **48**, 14130d (*synth*)

Caltrider, P.G. *et al., Antibiotics (N.Y.)*, 1967, **1**, 666-668 (*rev*)

Lokshin, G.B. *et al., Antibiotiki (Moscow)*, 1970, **15**, 14-18; *CA*, **72**, 109788a (*isol*)

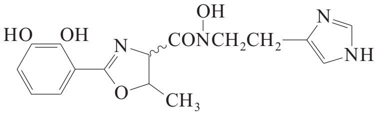
Eisenberg, M.A. *et al., Antimicrob. Agents Chemother.*, 1982, **21**, 5-10 (*activity*)

Nadkarni, R.S. *et al., J. Antibiot.*, 1983, **36**, 1567-1568 (*activity*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, CMP885

Acinetobactin A-79

[160472-93-5]



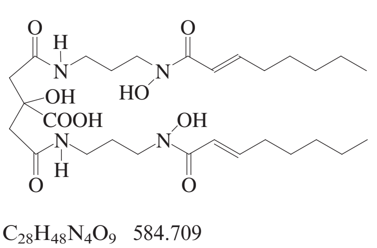
$C_{16}H_{18}N_4O_5$ 346.342

Closely related to Anguibactin, A-1009. Isol. from low-iron cultures of *Acinetobacter baumannii* ATCC 19606 and *Acinetobacter haemolyticus*. Siderophore. Sol. H_2O. λ_{max} 250; 317 (MeOH) (Berdy).

Yamamoto, S. *et al., Arch. Microbiol.*, 1994, **162**, 249 (*isol, pmr, cmr, ms*)

Acinetoferrin A-80

[156737-07-4]



$C_{28}H_{48}N_4O_9$ 584.709

Isol. from *Acinetobacter haemolyticus*. Siderophore.

Okujo, N. *et al., BioMetals*, 1994, **7**, 170-176 (*isol, pmr, cmr, ms*)

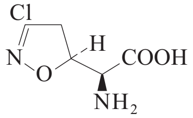
Wang, Q.X. *et al., J.O.C.*, 1998, **63**, 1491-1495 (*synth, pmr*)

Luo, M. *et al., J.A.C.S.*, 2005, **127**, 1726-1736 (*props*)

Acivicin, INN, USAN A-81

α-Amino-3-chloro-4,5-dihydro-5-isoxazoleacetic acid, 9CI. AT 125. NSC 163501. U 42126. Antibiotic AT 125. Antibiotic U 42126

[52583-41-2]



$C_5H_7ClN_2O_3$ 178.575

Amino acid antibiotic.

(αS,5S)-form [42228-92-2]

Prod. by *Streptomyces sviceus*. Antineoplastic agent. Cryst. (MeOH aq.). Sol. H_2O; fairly sol. MeOH; poorly sol. butanol, hexane. Mp 228-230°. $[\alpha]_{378}^{20}$ +135 (c, 0.159 in H_2O). Related to Ibotenic acid, I-8.

▶ NY2103000

4S-Hydroxy: ***Antibiotic U 43795***. *U 43795*

[54549-02-9]

$C_5H_7ClN_2O_4$ 194.574

From *Streptomyces sviceus*. Antineoplastic, antimetabolite. Sol. H_2O; poorly sol. Me_2CO, hexane.

Hanka, L.J. *et al., Antimicrob. Agents Chemother.*, 1973, **3**, 425; 1975, **7**, 807 (*isol, props*)

Martin, D.G. *et al., Tet. Lett.*, 1973, 2549 (*isol, abs config*)

Martin, D.G. *et al., J. Antibiot.*, 1975, **28**, 91 (*deriv*)

Kelly, R.C. *et al., J.A.C.S.*, 1979, **101**, 1054 (*synth*)

Silverman, R.B. *et al., J.A.C.S.*, 1981, **103**, 7357 (*synth*)

Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 12317

O'Dwyer, P.J. *et al., J. Clin. Oncol.*, 1984, **2**, 1064 (*rev, pharmacol*)

Earhart, W.D. *et al., Adv. Enzyme Regul.*, 1985, **24**, 179 (*rev, pharmacol*)

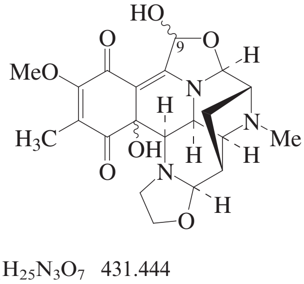
Baldwin, J.E. *et al., Tetrahedron*, 1985, **41**, 5241 (*synth, bibl*)

Mzengeza, S. *et al., J.O.C.*, 1988, **53**, 4074 (*synth, bibl*)

Cintas, P. *et al., Tetrahedron*, 1991, **47**, 6079 (*synth*)

Aclidinomycin B A-82

[342814-66-8]



$C_{21}H_{25}N_3O_7$ 431.444

Related to Naphthyridinomycin A, N-32. Prod. by *Streptomyces halstedi* KB012 and a marine-derived *Streptomyces* sp. $[\alpha]_D$ +188 (c, 0.16 in MeOH). λ_{max} 286 (ϵ 21500); 398 (ϵ 5000) (MeOH).

N*-De-Me:* ***Aclidinomycin D***

$C_{20}H_{23}N_3O_7$ 417.418

Prod. by a marine-derived *Streptomyces* sp.

9-Deoxy: ***Aclidinomycin A***

[342814-65-7]

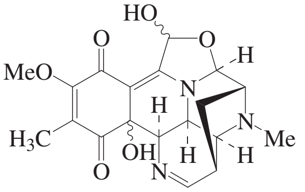
$C_{21}H_{25}N_3O_6$ 415.445

Prod. by *Streptomyces halstedi* KB012. $[\alpha]_D$ 0 (MeOH). λ_{max} 282 (ϵ 19000); 403 (ϵ 3500) (MeOH).

Thorwest, M. *et al., Dissertation*, Univ. of Göttingen, 2001, (*marine, isol*)

Cang, S. *et al., J. Antibiot.*, 2001, **54**, 304-307 (*isol, pmr, cmr*)

Aclidinomycin C A-83



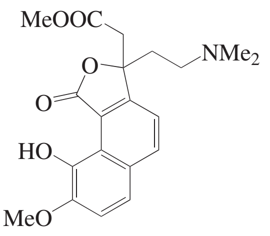
$C_{19}H_{21}N_3O_6$ 387.391

Prod. by a marine-derived *Streptomyces* sp.

Thorwest, M. *et al., Dissertation*, Univ. of Göttingen, 2001,

Aconcaguine A-84

[96624-39-4]

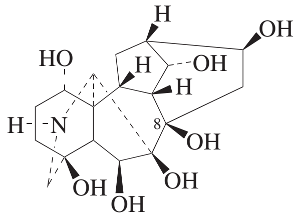


$C_{20}H_{23}NO_6$ 373.405

Alkaloid from the twigs of *Berberis actinacantha* (Berberidaceae). Yellow amorph. solid. Positive opt. rotn.

Weiss, I. *et al., Chem. Comm.*, 1985, 3-4 (*uv, ir, pmr, cmr, ms, struct*)

Aconitane-1,4,6,7,8,14,16-heptol A-85



$C_{18}H_{27}NO_7$ 369.414

(1α,5β,6β,14α,16β)-*form*

O^{6},O^{16}-*Di-Me,* N-*Et:* ***Delbine***†
[1356-54-3]
$C_{22}H_{35}NO_7$ 425.521
Alkaloid from the roots of *Delphinium bonvalotii* (Ranunculaceae). Mp 116-118°. $[\alpha]_D^{27}$ +53.3 (c, 0.1 in MeOH).

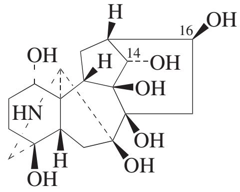
O^{1},O^{14},O^{16}-*Tri-Me,* N-*Et, 4*-O-*(2-acetamidobenzoyl):* ***Sinomontanine H***
$C_{32}H_{44}N_2O_9$ 600.708
Alkaloid from *Aconitum sinomontanum*. $[\alpha]_D^{17}$ -28.8 (c, 0.5 in $CHCl_3$).

O^{1},O^{6},O^{14},O^{16}-*Tetra-Me,* N-*Et, 8-Ac:* ***Hispaconitine***
[128581-45-3]
$C_{26}H_{41}NO_8$ 495.612
Alkaloid from the roots of *Aconitum barbatum* var. *hispidum* (Ranunculaceae). Mp 185-187°. $[\alpha]_D$ +43.4 (c, 1.19 in $CHCl_3$).

7-Hydroperoxide, O^{1},O^{6},O^{14},O^{16}-*tetra-Me,* N-*Et:* ***Lineariline***
$C_{24}H_{39}NO_8$ 469.574
Alkaloid from the roots of *Delphinium linearilobum*. Amorph. solid. $[\alpha]_D^{20}$ +18.4 (c, 0.5 in $CHCl_3$). λ_{max} 201 ($\log \epsilon$ 4); 226 (sh) ($\log \epsilon$ 3.1); 257 ($\log \epsilon$ 2.5) (MeOH).

Jiang, Q.P. *et al., Heterocycles*, 1985, **23**, 11 (*Delbine*)
Lao, A. *et al., Heterocycles*, 1990, **31**, 27 (*Hispaconitine*)
Peng, C.-S. *et al., Youji Huaxue*, 2005, **25**, 1235-1239; *CA*, **144**, 103949n (*Sinomontanine H*)
Kolak, U. *et al., Phytochemistry*, 2006, **69**, 2170-2175 (*Lineariline*)

Aconitane-1,4,7,8,9,14,16-heptol A-86



(1α,14α,16β)-*form*

$C_{18}H_{27}NO_7$ 369.414

(1α,14α,16β)-*form*

O^{14},O^{16}-*Di-Me,* N-*Et:* ***Sinomontanine E***
$C_{22}H_{35}NO_7$ 425.521
Alkaloid from the roots of *Aconitum sinomontanum*. $[\alpha]_D^{17}$ +7.8 (c, 0.5 in $CHCl_3$).

O^{1},O^{14},O^{16}-*Tri-Me, 4*-O-*(2-acetamidobenzoyl):* ***Sinomontanine F***
[872977-64-5]
$C_{30}H_{40}N_2O_9$ 572.654
Alkaloid from the roots of *Aconitum sinomontanum*. $[\alpha]_D^{17}$ +44.4 (c, 0.75 in $CHCl_3$).

O^{1},O^{14},O^{16}-*Tri-Me,* N-*Et:* ***Ranaconine.*** *Hydroxylappaconine*
[70474-32-7]
$C_{23}H_{37}NO_7$ 439.548
Alkaloid detected by glc-ms in *Aconitum leucostomum*. Alkaline hydrol. product of Ranaconitine (Ranunculaceae). Mp 107-109°.

O^{1},O^{14},O^{16}-*Tri-Me,* N-*Et, 4*-O-*(2-aminobenzoyl):* **N-*Deacetylranaconitine***
[82872-80-8]
$C_{30}H_{42}N_2O_8$ 558.67
Alkaloid from the roots of *Aconitum finetianum* (Ranunculaceae). Shows good analgesic activity. Mp 125-127°.

O^{1},O^{14},O^{16}-*Tri-Me,* N-*Et, 4*-O-*(2-acetamidobenzoyl):* ***Ranaconitine***
[1360-76-5]
$C_{32}H_{44}N_2O_9$ 600.708
Alkaloid from *Aconitum ranunculaefolium, Aconitum sinomontanum, Aconitum finetianum* and *Aconitum barbatum* var. *puberulum* (Ranunculaceae). Mp 132-134°. $[\alpha]_D^{27}$ +33.2 (c, 0.5 in $CHCl_3$).

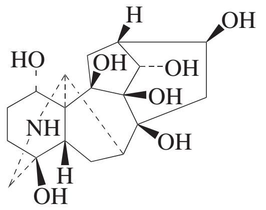
O^{1},O^{14},O^{16}-*Tri-Me, 4*-O-*(2-acetamidobenzoyl),* N-*Ac:* ***Sinaconitine A***
$C_{32}H_{42}N_2O_{10}$ 614.691
Alkaloid from the roots of *Aconitum sinomontanum*. Prisms (petrol/Et_2O). Mp 150-151.5°. $[\alpha]_D^{20}$ +35 (c, 1 in $CHCl_3$).

(1β,14α,16β)-*form*

O^{1},O^{14},O^{16}-*Tri-Me,* N-*Et, 4*-O-*(2-acetamidobenzoyl):* ***Puberanine***
[83685-20-5]
$C_{32}H_{44}N_2O_9$ 600.708
Alkaloid from the roots of *Aconitum barbatum* var. *puberulum* (Ranunculaceae). Amorph. $[\alpha]_D^{20}$ +16.6 (c, 0.6 in $CHCl_3$).

Mollov, N. *et al., Dokl. Bulg. Akad. Nauk*, 1964, **17**, 251; *CA*, **61**, 12324h (*Ranaconitine, isol, ir*)
Pelletier, S.W. *et al., Tet. Lett.*, 1978, 5045 (*Ranaconitine, pmr, cmr, struct*)
Pelletier, S.W. *et al., Can. J. Chem.*, 1979, **57**, 1652 (*cmr*)
Plugar, V.N. *et al., Khim. Prir. Soedin.*, 1982, **18**, 80; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 75 (*Ranaconine*)
Jiang, S. *et al., Yaoxue Xuebao*, 1982, **17**, 283; 1983, **18**, 440; *CA*, **97**, 20736a; **100**, 20505e (*Deacetylranaconitine*)
Yu, D. *et al., Planta Med.*, 1983, **49**, 85 (*Puberanine*)
Peng, C.-S. *et al., Yaoxue Xuebao*, 2000, **35**, 201-203 (*Sinomontanine E*)
Peng, C.-S. *et al., Youji Huaxue*, 2005, **25**, 1235-1239; *CA*, **144**, 103949n (*Sinomontanine F*)
Tan, J.-J. *et al., J. Asian Nat. Prod. Res.*, 2006, **8**, 535-539 (*Sinaconitine A*)

Aconitane-1,4,8,9,10,14,16-heptol A-87



$C_{18}H_{27}NO_7$ 369.414

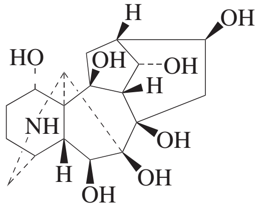
(1α,5β,14α,16β)-*form*

O^{1},O^{14},O^{16}-*Tri-Me,* N-*Et, 4*-O-*(2-aminobenzoyl):* ***Sepaconitine***
[114622-05-8]
$C_{30}H_{42}N_2O_8$ 558.67
Alkaloid from the aerial parts of *Aconitum septentrionale* (Ranunculaceae). Mp 250-253°. $[\alpha]_D^{20}$ +25 (c, 0.60 in $CHCl_3$).

O^{1},O^{14},O^{16}-*Tri-Me,* N-*Et, 4*-O-*(2-acetamidobenzoyl):* **N-*Acetylsepaconitine***
[118201-55-1]
$C_{32}H_{44}N_2O_9$ 600.708
Alkaloid from aerial parts of *Aconitum leucostomum* (Ranunculaceae). Amorph.

Usmanova, S.K. *et al., Khim. Prir. Soedin.*, 1987, **23**, 879; *Chem. Nat. Compd. (Engl. Transl.)*, 734 (*Sepaconitine*)
Tel'nov, V.A. *et al., Khim. Prir. Soedin.*, 1988, **24**, 556; *Chem. Nat. Compd. (Engl. Transl.)*, 472 (*N-Acetylsepaconitine*)

Aconitane-1,6,7,8,10,14,16-heptol A-88



$C_{18}H_{27}NO_7$ 369.414

(1α,5β,6β,14α,16β)-*form*

O^{1},O^{14},O^{16}-*Tri-Me,* N-*Et:* ***Acoseptrine***
[146028-66-2]
$C_{23}H_{37}NO_7$ 439.548
Alkaloid from roots of *Aconitum septentrionale*. Cryst. (Me_2CO/hexane). Mp 105-107°. $[\alpha]_D$ +19.6 (c, 0.245 in $CHCl_3$).

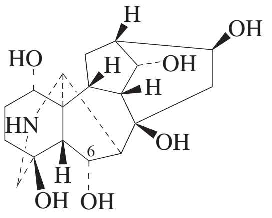
O^{7},O^{8}-*Methylene,* O^{1},O^{16}-*di-Me,* N-*Et, 6-Ac:* ***Anthriscifolcine C***
[948308-30-3]
$C_{25}H_{37}NO_8$ 479.569
Alkaloid from *Delphinium anthriscifolium* var. *savatieri*. Needles. Mp 222-224°. $[\alpha]_D^{20}$ -11.4 (c, 0.5 in $CHCl_3$).

O^{7},O^{8}-*Methylene,* O^{1},O^{14},O^{16}-*tri-Me,* N-*Et:* ***Anthriscifolcine E***
[948308-32-5]
$C_{24}H_{37}NO_7$ 451.559
Alkaloid from *Delphinium anthriscifolium* var. *savatieri*. Amorph. powder. Mp 150-152°. $[\alpha]_D^{20}$ -34.8 (c, 0.5 in $CHCl_3$).

O^{7},O^{8}-*Methylene,* O^{1},O^{14},O^{16}-*tri-Me,* N-*Et, 6-Ac:* ***Anthriscifolcine D***
[948308-31-4]
$C_{26}H_{39}NO_8$ 493.596
Alkaloid from *Delphinium anthriscifolium* var. *savatieri*. Amorph. powder. Mp 185-187°. $[\alpha]_D^{20}$ -41.3 (c, 0.5 in $CHCl_3$).

Sayed, H.M. *et al., J. Nat. Prod.*, 1992, **55**, 1595-1606 (*Acoseptrine*)
Song, L. *et al., Chem. Pharm. Bull.*, 2007, **55**, 918-921 (*Anthriscifolcines C-E*)

Aconitane-1,4,6,8,14,16-hexol A-89



(1α,5β,6α,14α,16β)-*form*

$C_{18}H_{27}NO_6$ 353.414

(1α,5β,6α,14α,16β)-*form*

O^{1},O^{6},$O^{14}O^{16}$-*Tetra-Me*, N-*Et*, *4-Ac*: ***Kirimine***
[161068-74-2]
$C_{26}H_{41}NO_7$ 479.612
Alkaloid from *Aconitum kirinense*.

(1α,5β,6β,14α,16β)-*form*

O^{6},O^{14},O^{16}*Tri-Me*, N-*Et*: ***Akiramidine***
[287724-50-9]
$C_{23}H_{37}NO_6$ 423.548
Alkaloid from the epigeal parts of *Aconitum kirinense*. Amorph. powder.

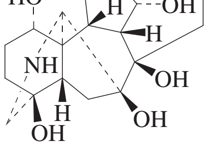
O^{6},O^{14},O^{16}-*Tri-Me*, N-*Et*, *4-Ac*: ***Akiramine***
[270073-83-1]
$C_{25}H_{39}NO_7$ 465.586
Alkaloid from the epigeal part of *Aconitum kirinense*. Cryst. (Me_2CO). Mp 162-164°.

O^{1},O^{6},O^{14},O^{16}-*Tetra-Me*, N-*Et*: ***Akiranine***
[213478-70-7]
$C_{24}H_{39}NO_6$ 437.575
Alkaloid from *Aconitum kirinense*. Amorph. Mp 102-104°.

O^{1},O^{6},O^{14},O^{16}-*Tetra-Me*, N-*Et*, *4-Ac*: ***Akirane***
[171119-09-8]
$C_{26}H_{41}NO_7$ 479.612
Alkaloid from aerial parts of *Aconitum kirinense*. Cryst. (Me_2CO). Mp 214-217°.

Sultankhodzhaev, M.N. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1994, **30**, 603; 1997, **33**, 700-701 (*Akirane, Akiranine*)
Feng, F. *et al., CA*, 1995, **122**, 128605f (*Kirimine*)
Teshebaeva, U.T. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1999, **35**, 445-447; 659-660 (*Akiramidine, Akiramine*)

Aconitane-1,4,7,8,14,16-hexol A-90



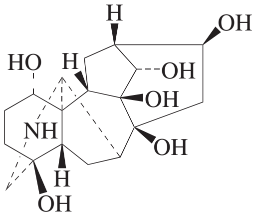
$C_{18}H_{27}NO_6$ 353.414

(1α,5β,14α,16β)-*form*

O^{1},O^{14},O^{16}-*Tri-Me*, N-*Et*, 4-O-*(2-acetamidobenzoyl)*: ***Isolappaconitine***
[114216-94-3]
$C_{32}H_{44}N_2O_8$ 584.708
Alkaloid from the roots of *Aconitum finetianum* (Ranunculaceae) and *Aconitum rubicundum*. Cryst (Et_2O). Mp 186-188°.

Jiang, S. *et al., Huaxue Xuebao*, 1988, **46**, 26; *CA*, **108**, 183673n (*Isolappaconitine*)
Nishanov, A.A. *et al., Khim. Prir. Soedin.*, 1991, **27**, 403-407; *Chem. Nat. Compd. (Engl. Transl.)*, 352, **1991**, 27-349 (*Isolappaconitine, isol, pmr, ms*)

Aconitane-1,4,8,9,14,16-hexol A-91



$C_{18}H_{27}NO_6$ 353.414

(1α,5β,14α,16β)-*form*

O^{14},O^{16}-*Di-Me*, N-*Et*: ***Lappaconidine***. *Lapaconidine*
[31000-13-2]
$C_{22}H_{35}NO_6$ 409.522
Alkaloid from the roots of *Aconitum leucostomum* (*Aconitum excelsum*) (Ranunculaceae). Mp 206-207°. $[\alpha]_D$ +12.9 ($CHCl_3$). Forms benzene solvate, Mp 118-120°.

O^{14},O^{16}-*Di-Me*, N-*Et*, *tetra-Ac*: Mp 195-197°.

O^{14},O^{16}-*Di-Me*, N-*Et*, 4-O-*(2-aminobenzoyl)*: ***4-Anthranoyllappaconidine***
[139441-64-8]
$C_{29}H_{40}N_2O_7$ 528.644
Alkaloid from roots of *Aconitum septentrionale* (Ranunculaceae). Amorph. $[\alpha]_D$ +48.8 (c, 0.16 in $CHCl_3$).

O^{14},O^{16}-*Di-Me*, N-*Et*, 4-O-*(2-acetamidobenzoyl)*: ***1-De-O-methyllappaconitine***. *Sinomontanine B*
[139085-68-0]
$C_{31}H_{42}N_2O_8$ 570.681
Alkaloid from *Aconitum orientale* and *Aconitum sinomontanum*. Powder. $[\alpha]_D$ +52 (c, 0.1 in $CHCl_3$).

O^{1},O^{14},O^{16}-*Tri-Me*, 4-O-*(2-acetamidobenzoyl)*: ***Sinomontanine A***
$C_{30}H_{40}N_2O_8$ 556.655
Alkaloid from the roots of *Aconitum sinomontanum*. Amorph. powder. $[\alpha]_D$ +31.2 (c, 0.5 in $CHCl_3$).

O^{1},O^{14},O^{16}-*Tri-Me*, N-*Ac*, 4-O-*(2-acetamidobenzoyl)*: ***Sinaconitine B***
$C_{32}H_{42}N_2O_9$ 598.692
Alkaloid from the roots of *Aconitum sinomontanum*. Amorph. powder. $[\alpha]_D^{20}$ +17 (c, 0.35 in $CHCl_3$).

O^{1},O^{14},O^{16}-*Tri-Me*, N-*Et*: ***Lappaconine***
[23943-93-3]
$C_{23}H_{37}NO_6$ 423.548
Detected in *Aconitum leucostomum* (Ranunculaceae). Cryst. + 1½ H_2O (H_2O). Mp 96°. $[\alpha]_D^{25}$ +27 (c, 3.17 in $CHCl_3$).

▶ AR5569540

O^{1},O^{14},O^{16}-*Tri-Me*, N-*Et*, 4-O-*(2-aminobenzoyl)*: ***Puberanidine***. N-*Deacetyllappaconitine*
[11033-64-0]
$C_{30}H_{42}N_2O_7$ 542.671
Alkaloid from *Aconitum ranunculaefolium* and from the roots of *Aconitum barbatum* var. *puberulum, Aconitum septentrionale, Aconitum finetianum* and *Delphinium cashmirianum* (Ranunculaceae). Prisms (MeOH), needles (Me_2CO/hexane), or amorph. Mp 213-214.5° (120-121°, 209-214°). $[\alpha]_D^{20}$ +23.2 (c, 0.9 in $CHCl_3$) (for amorph. product). $[\alpha]_D^{27}$ +42 (c, 0.34 in EtOH).

▶ OE5784120

O^{1},O^{14},O^{16}-*Tri-Me*, N-*Et*, 4-O-*(2-acetamidobenzoyl)*: ***Lappaconitine***
[32854-75-4]
$C_{32}H_{44}N_2O_8$ 584.708
Alkaloid from *Aconitum septentrionale, Aconitum orientale, Aconitum excelsum, Aconitum sinomontanum, Aconitum finetianum, Aconitum ranunculaefolium, Aconitum barbatum* var. *puberulum* and *Delphinium cashmirianum* (Ranunculaceae). Cryst. (Et_2O). Mp 227° (219-221°). $[\alpha]_D^{25}$ +28.2 (c, 2.07 in $CHCl_3$).

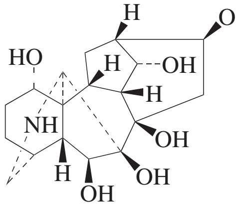
▶ OE5784100

O^{1},O^{14},O^{16}-*Tri-Me*, N-*Et*, 4-O-*(2-methylaminobenzoyl)*: ***Septefine***. *Septephine*
$C_{31}H_{44}N_2O_7$ 556.698
Alkaloid from *Aconitum septentrionale* (Ranunculaceae). Cryst. (MeOH). Mp 194-195°.

Mollov, N. *et al., Dokl. Bulg. Akad. Nauk*, 1964, **17**, 251; *CA*, **61**, 12324h (*Puberanidine, isol, struct*)
Khamova, M. *et al., Tet. Lett.*, 1964, 2711 (*Lappaconidine, Lappaconitine, ir, pmr, struct*)
Marion, L. *et al., Can. J. Chem.*, 1967, **45**, 969 (*Lappaconidine, Lappaconitine, isol, ir, pmr, struct*)
Mollov, N. *et al., Tet. Lett.*, 1969, 2189 (*Lappaconidine, pmr, struct*)
Birnbaum, G.I. *et al., Acta Cryst. B*, 1970, **26**, 755 (*Lappaconine, cryst struct*)
Tel'nov, V.A. *et al., Khim. Prir. Soedin.*, 1970, **6**, 583; 1971, **7**, 622; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 598; 1971, **7**, 601 (*Lappaconidine, Lappaconitine*)
Pelletier, S.W. *et al., Can. J. Chem.*, 1979, **57**, 1652 (*cmr*)
Shamma, M. *et al., J. Nat. Prod.*, 1979, **42**, 615 (*Puberanidine, isol, ir, pmr, struct*)
Plugar, V.N. *et al., Khim. Prir. Soedin.*, 1982, **18**, 80; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 75 (*Lappaconidine, glc, ms*)
Yu, D. *et al., Planta Med.*, 1983, **49**, 85 (*Puberanidine, uv, ir, pmr, cmr, ms, struct*)
Sayed, H.M. *et al., J. Nat. Prod.*, 1992, **55**, 1595 (*4-Anthranoyllappaconidine*)
Usmanova, S.K. *et al., Khim. Prir. Soedin.*, 1996, **32**, 225-228; *Chem. Nat. Compd. (Engl. Transl.)*, 1996, **32**, 198-200 (*Septefine*)

Ulubelen, A. *et al., Phytochemistry*, 1996, **41**, 957 (*1-Demethyllappaconitine*)
Wang, F.-P. *et al., J. Asian Nat. Prod. Res.*, 2001, **3**, 15-22 (*Sinomontanines*)
Tan, J.J. *et al., J. Asian Nat. Prod. Res.*, 2006, **8**, 535-539 (*Sinaconitine B*)
Wang, Y.-P. *et al., Acta Cryst. E*, 2007, **63**, o1645-o1647 (*Lappaconitine, cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LBD000

Aconitane-1,6,7,8,14,16-hexol A-92



$C_{18}H_{27}NO_6$ 353.414

(1α,5β,6β,14α,16β)-*form*

O¹,O¹⁴,O¹⁶-Tri-Me, N-*Et: Umbrophine. Umbrofine.* ***Acosepticine***
[144049-71-8]
$C_{23}H_{37}NO_6$ 423.548
Alkaloid from roots of *Aconitum septentrionale* and *Aconitum umbrosum* (Ranunculaceae). Amorph. solid. $[\alpha]_D$ +23.4 (c, 0.385 in $CHCl_3$). Identity with Umbrophine (cryst., Mp. 110-112°, no opt. rotn. reported) is tentative.

O¹,O¹⁴,O¹⁶-Tri-Me, N-*Et, 6-Ac:* ***6-O-Acetylacosepticine****. 6-Acetylumbrophine*
[144074-85-1]
$C_{25}H_{39}NO_7$ 465.586
Alkaloid from roots of *Aconitum septentrionale* and *Aconitum umbrosum* (Ranunculaceae). Cryst. (Et_2O). Mp 168.5-170.5°. $[\alpha]_D$ -1.2 (c, 0.2 in $CHCl_3$).

O¹,O⁶,O¹⁴,O¹⁶-Tetra-Me, N-*Et:* ***Exceconidine***
$C_{24}H_{39}NO_6$ 437.575
Alkaloid from *Aconitum excelsum*. Powder.

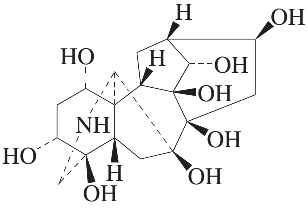
O⁷,O⁸-Methylene, O¹,O¹⁴,O¹⁶*-tri-Me,* N-*Et:* ***Anthriscifolcine B***
[948308-29-0]
$C_{24}H_{37}NO_6$ 435.559
Alkaloid from *Delphinium anthriscifolium* var. *savatieri*. Amorph. powder. Mp 75-77°. $[\alpha]_D^{20}$ -27 (c, 0.5 in $CHCl_3$).

O⁷,O⁸-Methylene, O¹,O¹⁴,O¹⁶*-tri-Me,* N-*Et, 6-Ac:* ***Anthriscifolcine A***
[948308-28-9]
$C_{26}H_{39}NO_7$ 477.597
Alkaloid from *Delphinium anthriscifolium* var. *savatieri*. Amorph. powder. Mp 135-137°. $[\alpha]_D^{20}$ -12.2 (c, 0.5 in $CHCl_3$).

6-Ketone, O¹,O¹⁴,O¹⁶*-tri-Me,* N-*Et:* ***Leucostine***
[192386-08-6]
$C_{23}H_{35}NO_6$ 421.533
Alkaloid from *Aconitum leucostomum*. $[\alpha]_D^{25}$ +19.4 (c, 0.05 in EtOH). Not to be confused with Leucostine A in M-309.

Sayed, H.M. *et al., J. Nat. Prod.*, 1992, **55**, 1595 (*Acosepticine*)
Ross, S.A. *et al., Tetrahedron*, 1992, **48**, 1183 (*6-O-Acetylacosepticine*)
Tel'nov, V.A. *et al., Khim. Prir. Soedin.*, 1993, **29**, 73-77; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 60-63 (*Umbrofine, 6-Acetylumbrofine*)
Wei, X. *et al., Zhiwu Xuebao (Acta Bot. Sin.)*, 1996, **38**, 995-997; *CA*, **127**, 147062w (*Leucostine*)
Zhang, S.X. *et al., Chin. Chem. Lett.*, 1999, **10**, 133-134 (*Exceconidine*)
Zinurova, E.G. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2000, **36**, 387-389 (*Leucostine*)
Song, L. *et al., Chem. Pharm. Bull.*, 2007, **55**, 918-921 (*Anthriscifolcines A,B*)

Aconitane-1,3,4,7,8,9,14,16-octol A-93



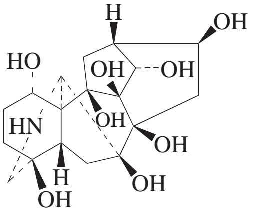
$C_{18}H_{27}NO_8$ 385.413

(1α,3α,14α,16β)-*form*

O¹⁴,O¹⁶-Di-Me, N-*Et:* ***Sinomontanine D***
$C_{22}H_{35}NO_8$ 441.52
Alkaloid from the roots of *Aconitum sinomontanum*. $[\alpha]_D^{17}$ +26.6 (c, 0.5 in $CHCl_3$).

Peng, C. *et al., Yaoxue Xuebao*, 2000, **35**, 201-203

Aconitane-1,4,7,8,9,10,14,16-octol A-94



$C_{18}H_{27}NO_8$ 385.413

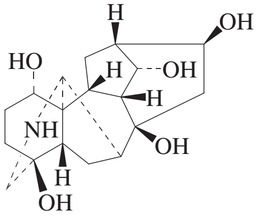
(1α,5β,14α,16β)-*form*

O¹,O¹⁴,O¹⁶-Tri-Me, N-*Et, 4-*O-*(2-aminobenzoyl):* **N-*Deacetylfinaconitine***
[82872-81-9]
$C_{30}H_{42}N_2O_9$ 574.67
Alkaloid from the roots of *Aconitum finetianum* (Ranunculaceae). Mp 121-123°.

O¹,O¹⁴,O¹⁶-Tri-Me, N-*Et, 4-*O-*(2-acetamidobenzoyl):* ***Finaconitine****. 10-Hydroxyranaconitine*
[81161-27-5]
$C_{32}H_{44}N_2O_{10}$ 616.707
Alkaloid from the roots of *Aconitum finetianum* (Ranunculaceae). Mp 220-221°.

Jiang, S. *et al., Yaoxue Xuebao*, 1982, **17**, 283; 1983, **18**, 440; *CA*, **97**, 20736a; **100**, 20505e (*Finaconitine, Deacetylfinaconitine*)

Aconitane-1,4,8,14,16-pentol A-95



$C_{18}H_{27}NO_5$ 337.415

(1α,5β,14α,16β)-*form*

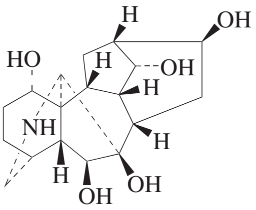
O¹⁴,O¹⁶-Di-Me, N-*Et:* ***Dihydromonticamine***
[81037-23-2]
$C_{22}H_{35}NO_5$ 393.522
Alkaloid from the aerial parts of *Aconitum monticola* (Ranunculaceae). Cryst. (Et_2O/Me_2CO). Mp 156-157°.

O¹,O¹⁴,O¹⁶-Tri-Me, N-*Et, 4-*O-*(2-aminobenzoyl):* ***Neofinaconitine****. Delphicrispuline*
[114244-02-9]
$C_{30}H_{42}N_2O_6$ 526.672
Alkaloid from the roots of *Aconitum finetianum* and *Delphinium crispulum* (Ranunculaceae). $[\alpha]_D^{20}$ +23.8 (c, 0.8 in $CHCl_3$) (Delphicrispuline).

O¹,O¹⁴,O¹⁶-Tri-Me, N-*Et, 4-*O-*(2-acetamidobenzoyl):* ***9-Deoxylappaconitine***
[114216-95-4]
$C_{32}H_{44}N_2O_7$ 568.709
Alkaloid from roots of *Aconitum finetianum* (Ranunculaceae).

Ametova, E.F. *et al., Khim. Prir. Soedin.*, 1982, 504; *Chem. Nat. Compd. (Engl. Transl.)*, 472 (*Dihydromonticamine*)
Jiang, S. *et al., Huaxue Xuebao*, 1988, **46**, 26; *CA*, **108**, 183673n (*Neofinaconitine, 9-Deoxylappaconitine*)
Ulubelen, A. *et al., Phytochemistry*, 1999, **50**, 513-516 (*Delphicrispuline*)

Aconitane-1,6,7,14,16-pentol A-96



$C_{18}H_{27}NO_5$ 337.415

(1α,5β,14α,16β)-*form*

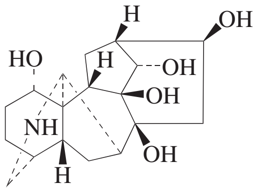
6-Ketone, O¹,O¹⁴,O¹⁶*-tri-Me,* N-*Et:* ***Leuconine***
[192386-06-4]
$C_{23}H_{35}NO_5$ 405.533

Alkaloid from *Aconitum leucostomum*. Cryst. (Me_2CO/hexane). Mp 195-197°.

Tel'nov, V.A. *et al., Khim. Prir. Soedin.*, 1992, **28**, 538-540; *Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 470-471 (*isol, ms, cmr*)

Wei, X. *et al., Zhiwu Xuebao (Acta Bot. Sin.)*, 1996, **38**, 995-997; *CA*, **127**, 147062w (*isol*)

Aconitane-1,8,9,14,16-pentol A-97



$C_{18}H_{27}NO_5$ 337.415

(1α,5β,14α,16β)-*form*

O^{1},O^{16}-*Di-Me,* N-*Et:* **Episcopalisinine**

[83692-39-1]

$C_{22}H_{35}NO_5$ 393.522

Alkaloid from the roots of *Aconitum episcopale* (Ranunculaceae).

O^{1},O^{16}-*Di-Me,* N-*Et, 14-benzoyl:* **Episcopalisine**. *14-Benzoylepiscopalisinine*

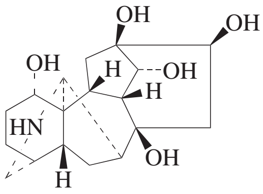
[83685-22-7]

$C_{29}H_{39}NO_6$ 497.63

Alkaloid from the roots of *Aconitum episcopale* (Ranunculaceae).

Wang, F. *et al., Yaoxue Xuebao*, 1983, **18**, 514-521; *CA*, **100**, 64981m (*Episcopalisinine, Episcopalisine*)

Aconitane-1,8,13,14,16-pentol A-98



$C_{18}H_{27}NO_5$ 337.415

(1α,5β,14α,16β)-*form*

O^{1},O^{16}-*Di-Me,* N-*Et, 14-Ac:* **Delavaconitine F**

[1022894-28-5]

$C_{24}H_{37}NO_6$ 435.559

Alkaloid from the roots of *Aconitum delavayi*. Amorph. powder.

O^{1},O^{16}-*Di-Me,* N-*Et, 14-benzoyl:* **Delavaconitine**

[1356-52-1]

$C_{29}H_{39}NO_6$ 497.63

Alkaloid from the roots of the Chinese drug Tzu-Tsao-Wu (*Aconitum delavayi*). Anaesthetic. Mp 241° (as perchlorate). Log P 0.24 (uncertain value) (calc).

▸AR5566000

O^{1},O^{16}-*Di-Me,* N-*Et, 14-benzoyl, 13-Ac:* **Delavaconitine E**

[126262-74-6]

$C_{31}H_{41}NO_7$ 539.667

Alkaloid from *Aconitum delavayi* (Ranunculaceae).

O,^{1}O^{16}-*Di-Me,* N-*Et, 14-*O*-(4-methoxybenzoyl):* **Contortumine**

[131653-96-8]

$C_{30}H_{41}NO_7$ 527.656

Alkaloid from the roots of *Aconitum contortum* (Ranunculaceae). Amorph. $[\alpha]_D$ -4.8 (c, 0.97 in EtOH).

Chu, J.-H. *et al., Huaxue Xuebao*, 1959, **25**, 321; *CA*, **54**, 17440i (*Delavaconitine*)

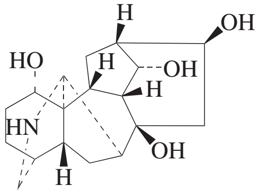
Zhu, Y. *et al., Heterocycles*, 1982, **17**, 607-644 (*Delvaconitine*)

Jiang, S. *et al., Huaxue Xuebao*, 1989, **47**, 1178; *CA*, **112**, 175625r (*Delvaconitine E*)

Niitsu, K. *et al., Heterocycles*, 1990, **31**, 1517-1524 (*Contortumine*)

Jiang, S.H. *et al., Chin. Chem. Lett.*, 2007, **18**, 409-411 (*Delavaconitines E,F*)

Aconitane-1,8,14,16-tetrol A-99



$C_{18}H_{27}NO_4$ 321.416

(1α,5β,14α,16β)-*form*

O^{16}-*Me,* N-*Et:* **Scopaline**

[80787-49-1]

$C_{21}H_{33}NO_4$ 363.496

Alkaloid from *Aconitum episcopale* (Ranunculaceae).

O^{1},O^{16}-*Di-Me,* N-*Et:* **Aconosine**

[38839-95-1]

$C_{22}H_{35}NO_4$ 377.523

Alkaloid from *Aconitum nasutum* (all parts of the plant), the aerial parts and roots of *Aconitum fischeri*, the foliage and roots of *Aconitum arcuatum*, and from the roots of *Aconitum forrestii, Aconitum napellus* and *Aconitum stapfianum* var. *pubipes* (Ranunculaceae). Cryst. (MeOH aq.). Mp 150° (148°). $[\alpha]_D$ -25 (c, 0.57 in MeOH). $[\alpha]_D^{20}$ -21 (c, 1 in MeOH).

▸AR5540000

O^{1},O^{16}-*Di-Me,* N-*Et, 14-Ac:* **Episcopalitine**. *Dolaconine*

[82841-75-6]

$C_{24}H_{37}NO_5$ 419.56

Alkaloid from the roots of *Aconitum episcopale* and *Aconitum stapfianum* var. *pubipes* (Ranunculaceae). Mp 44-46°.

O^{1},O^{16}-*Di-Me,* N-*Et, 8,14-di-Ac:* **8-Acetyldolaconine**. *8,14-Diacetylaconosine*

[132160-38-4]

$C_{26}H_{39}NO_6$ 461.597

Alkaloid from the roots of *Aconitum campylorrhynchum* (Ranunculaceae).

O^{1},O^{16}-*Di-Me,* N-*Et, 14-benzoyl:* **Delavaconitine C**

[126234-20-6]

$C_{29}H_{39}NO_5$ 481.631

Alkaloid from *Aconitum delavayi* (Ranunculaceae).

O^{1},O^{16}-*Di-Me,* N-*Et, 14-benzoyl, 8-Ac:* **Delavaconitine D**

[126234-21-7]

$C_{31}H_{41}NO_6$ 523.668

Alkaloid from *Aconitum delavayi* (Ranunculaceae).

Murav'eva, D.A. *et al., Khim. Prir. Soedin.*, 1972, **8**, 128-129; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 132-133 (*Aconosine, isol, ir, pmr, ms, struct*)

Yang, C. *et al., Huaxue Xuebao*, 1981, **39**, 445-452; *CA*, **96**, 82689a (*Scopaline*)

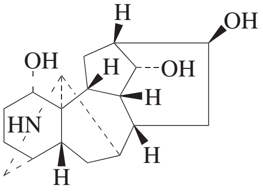
Luo, S. *et al., Huaxue Xuebao*, 1981, **39**, 808-810; *CA*, **97**, 107079n (*Aconosine, Dolaconine*)

Edwards, O.E. *et al., Can. J. Chem.*, 1983, **61**, 1194-1196 (*synth, ir, pmr, cmr, ms*)

Wang, F. *et al., Yaoxue Xuebao*, 1983, **18**, 514-521; *CA*, **100**, 64981m (*Episcopalitine*)

Ding, L.S. *et al., Yaoxue Xuebao*, 1990, **25**, 441-444; *CA*, **114**, 98113 (*8-Acetyldelaconine*)

Aconitane-1,14,16-triol A-100



$C_{18}H_{27}NO_3$ 305.416

(1α,5β,14α,16β)-*form*

*8-*O*-[2-(4-Hydroxyphenyl)ethoxy],* O^{1},O^{16}-*di-Me,* N-*Et:* **Piepunendine B**

[947321-59-7]

$C_{30}H_{43}NO_5$ 497.673

Alkaloid from the roots of *Aconitum piepunense*. Mp 85-87°. $[\alpha]_D^{20}$ -10.6 (c, 0.5 in $CHCl_3$).

14-Ketone, O^{1},O^{16}-*di-Me,* N-*Et:* **8-Deoxy-14-dehydroaconosine**

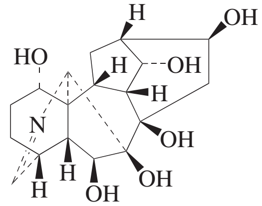
$C_{22}H_{33}NO_3$ 359.508

Alkaloid from *Aconitum stapfianum* (Ranunculaceae).

Liang, X.-T. *et al., Pure Appl. Chem.*, 1986, **58**, 711-718 (*rev*)

Cai, L. *et al., Nat. Prod. Commun.*, 2006, **1**, 191-194 (*Piepunendine B*)

Aconit-19(*N*)-ene-1,6,7,8,14,16-hexol A-101



$C_{18}H_{25}NO_6$ 351.399

(1α,5β,14α,16β)-*form*

O^{1},O^{6},O^{14},O^{16}-*Tetra-Me:* **Lamarckinine**†

[150375-24-9]

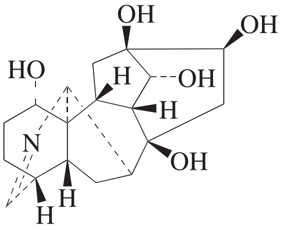
$C_{22}H_{33}NO_6$ 407.506

Alkaloid from aerial parts of *Aconitum lamarckii* (Ranunculaceae). Resin. $[\alpha]_D$ +76.6 (c, 1.1 in $CHCl_3$).

de la Fuente, G. *et al., Heterocycles*, 1993, **36**, 1455 (*isol, ir, pmr, cmr, ms, struct*)

Aconit-19(*N*)-ene-1,8,13,14,16-pentol

A-102



$C_{18}H_{25}NO_5$ 335.399

(1α,5β,14α,16β)-*form*

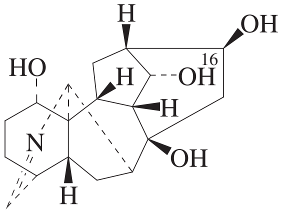
O^1,O^{16}-Di-Me, 14-benzoyl, 8,13-di-Ac: ***Delavaconitine G***
[1022894-29-6]
$C_{31}H_{37}NO_8$ 551.635
Alkaloid from the roots of *Aconitum delavayi*. Cryst. Mp 232-233°.

Jiang, S.H. *et al., Chin. Chem. Lett.*, 2007, **18**, 409-411 (*isol, pmr, cmr*)

Aconit-19(*N*)-ene-1,8,14,16-tetrol

A-103

19,20-Didehydroaconitane-1,8,14,16-tetrol



$C_{18}H_{25}NO_4$ 319.4

(1α,5β,14α,16β)-*form*

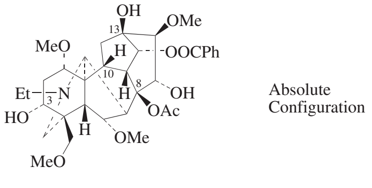
O^1,O^{16}-Di-Me: ***Liconosine A***
[126621-43-0]
$C_{20}H_{29}NO_4$ 347.453
Alkaloid from *Aconitum forrestii* (Ranunculaceae).

Chen, S. *et al., Yunnan Zhiwu Yanjiu*, 1989, **11**, 267; *CA*, **112**, 175578

Aconitine

A-104

[302-27-2]



$C_{34}H_{47}NO_{11}$ 645.745
Alkaloid from *Aconitum napellus, Aconitum fauriei, Aconitum grossedentatum, Aconitum hakusanense, Aconitum mokchangense, Aconitum zuccarini, Aconitum bullatifolium* var. *homotrichum, Aconitum carmichaeli, Aconitum karakolicum* and many others (Ranunculaceae). Toxic agent implicated in poisoning by *Aconitum* spp., esp. *Aconitum chasmanthum* in India, exp. arrhythmia effects. Gastric anaesthetic. Homeopathic remedy against neuralgia and febrile diseases. Cryst. V. spar. sol. H_2O. Mp 204°. $[\alpha]_D$ +19 ($CHCl_3$). pK_a 8.35 (15°). Hydrol. to 4-Methylaconitane-1,3,6,8,13,14,15,16,18-nonol, M-331.

▶ Very toxic if swallowed or by skin absorption. Human systemic effects by ingestion. LD_{50} (mus, orl) 1 mg/kg, LD_{50} (mus, ivn) 0.175 mg/kg, exp. lethal doses by subcutaneous route reported; LD_{50} (mus, ipr) 0.328 mg/kg. AR5960000

Hydrochloride: Mp 170-172° dec. $[\alpha]_D$ -31 (H_2O).

3-Ac: ***Flaconitine***. *3-Acetylaconitine*
[77181-26-1]
$C_{36}H_{49}NO_{12}$ 687.783
Alkaloid from the roots of *Aconitum flavum* and *Aconitum pendulum* (Ranunculaceae). Mp 196-197°. $[\alpha]_D^{24}$ +18.6 (c, 1 in $CHCl_3$).

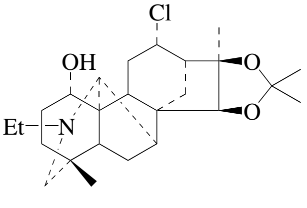
▶ AR5562000

Przybylska, M. *et al., Can. J. Chem.*, 1959, **37**, 1116-1118; 1843-1845 (*struct*)
Wiesner, K. *et al., Tet. Lett.*, 1959, **2**, 15-24 (*struct*)
Bachelor, F.W. *et al., Tet. Lett.*, 1960, **31**, 1-9 (*struct*)
Birnbaum, K.B. *et al., Tet. Lett.*, 1971, 867-870 (*config, struct*)
Chang, X. *et al., Yaoxue Xuebao*, 1981, **16**, 474-476; *CA*, **97**, 3590f (*Flaconitine, isol*)
Wang, H. *et al., Heterocycles*, 1985, **23**, 803-807 (*Flaconitine, cmr*)
Seeger, R. *et al., Dtsch. Apoth. -Ztg.*, 1994, **134**, 43-50; 53-54; *CA*, **121**, 308035 (*pharmacol, rev*)
Chan, T.Y. *et al., Vet. Hum. Toxicol.*, 1994, **36**, 326-328 (*pharmacol, rev*)
Ho, K. *et al., Planta Med.*, 1997, **63**, 75-79 (*ms*)
Ohta, H. *et al., J. Chromatogr., B*, 1998, **714**, 215-221 (*hplc, ms*)
Chen, Y. *et al., J. Nat. Prod.*, 1999, **62**, 701-704 (*isol, ms*)
Wang, Z. *et al., Fenxi Huaxue*, 2001, **29**, 391-395; *CA*, **135**, 127303 (*ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, ADH750

Acophine

A-105

Acofine
[169626-13-5]



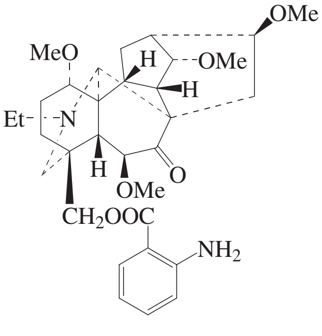
$C_{25}H_{38}ClNO_3$ 436.033
Alkaloid from roots of *Aconitum karakolicum*. Cryst. (Me_2CO). Mp 159-160°. Poss. artifact.

Tashkhodzhaev, B. *et al., Khim. Prir. Soedin.*, 1993, **29**, 267; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 222

Acoseptine

A-106

[257860-39-2]



$C_{32}H_{44}N_2O_7$ 568.709
Unusual (7→8)abeoaconitane skeleton. Alkaloid from the roots of *Aconitum septentrionale*. Cryst. (MeOH). Mp 127-128°.

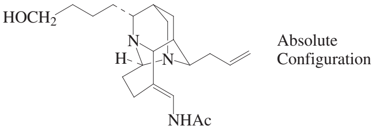
N-Succinimide: ***Anhydrolycaconitine***
[321554-91-0]
$C_{36}H_{46}N_2O_9$ 650.767
Alkaloid from the roots of *Aconitum septentrionale*. Cryst. (Me_2CO). Mp 215-216°. $[\alpha]_D^{20}$ +21 (c, 0.1 in $CHCl_3$). Misleading name.

Usmanova, S.K. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1999, **35**, 91-93 (*Acoseptine*)
Yunusov, M.S. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2000, **49**, 1629-1633 (*Anhydrolycaconitine*)
Khairitdinova, E.D. *et al., Russ. J. Org. Chem. (Engl. Transl.)*, 2008, **44**, 536-541 (*Anhydrolycaconitine*)

Acosmine

A-107

[250343-47-6]



$C_{21}H_{33}N_3O_2$ 359.511
Alkaloid from *Acosmium panamense* and *Bowdichia virgilioides*. Amorph. yellow solid. $[\alpha]_D$ -10.8 (c, 1.3 in $CHCl_3$). λ_{max} 242 ; 290 (sh) (MeOH).

O-Ac: ***Acosmine acetate***. *O-Acetylacosmine*
[250279-26-6]
$C_{23}H_{35}N_3O_3$ 401.548
Alkaloid from the seeds of *Acosmium panamense*. Amorph. yellow solid. $[\alpha]_D$ -15.7 (c, 0.86 in $CHCl_3$). λ_{max} 242 ; 290 (sh) (MeOH).

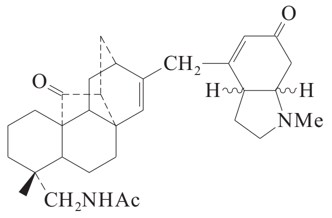
O-(3,4,5-Trimethoxybenzoyl): ***Bowdichine***
[730992-48-0]
$C_{31}H_{43}N_3O_6$ 553.697

Alkaloid from the stem bark of *Bowdichia virgilioides*. Viscous oil. λ_{max} 225 ; 250 ; 298 (MeOH).

Nuzillard, J.-M. *et al., Tetrahedron*, 1999, **55**, 11511-11518 (*Acosmine*)
Barbosa-Filho, J.M. *et al., J. Asian Nat. Prod. Res.*, 2004, **6**, 11-17 (*Bowdichine, pmr, cmr*)

Acozerine **A-108**

[155210-48-3]

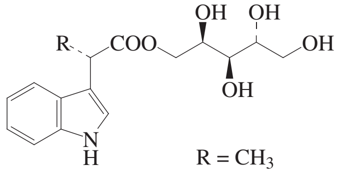


$C_{31}H_{42}N_2O_3$ 490.684
Alkaloid from *Aconitum zeravshanicum* (Ranunculaceae).

Vaisov, Z.M. *et al., Mendeleev Commun.*, 1993, 237; *CA*, **120**, 299052m (*isol, ir, pmr, ms*)

Acremoauxin A **A-109**

2-(3-Indolyl)propanoyl-D-arabinitol
[125537-93-1]



$C_{16}H_{21}NO_6$ 323.345
Prod. by *Acremonium roseum*. Plant growth regulator. Needles (EtOH/EtOAc). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 142-144° (135-136°). $[\alpha]_D^{19}$ +53.6 (c, 0.35 in MeOH). λ_{max} 219 (ϵ 25000); 225 (ϵ 9600); 278 (ϵ 7000); 286 (ϵ 5700); 288 (ϵ 6000) (MeOH) (Berdy).

Sassa, T. *et al., Agric. Biol. Chem.*, 1989, **53**, 3105 (*isol, struct*)
Yoshida, N. *et al., Agric. Biol. Chem.*, 1990, **54**, 2681 (*synth*)

Acremoauxin B **A-110**

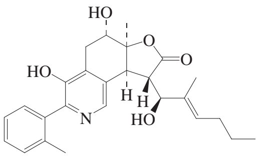
3-Indolylacetyl-D-arabinitol, 9CI
[138111-07-6]
As Acremoauxin A, A-109 with R = H

$C_{15}H_{19}NO_6$ 309.318
Prod. by *Acremonium roseum*. Plant growth regulator. Cryst.

Japan. Pat., 1991, 91 83 968; *CA*, **116**, 39794a

Acremolactone B **A-111**

[850723-60-3]



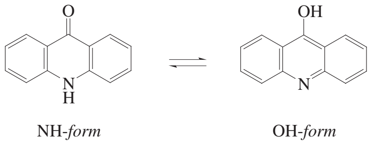
Absolute Configuration

$C_{26}H_{31}NO_5$ 437.535
Prod. by *Acremonium roseum* I4267. Phytotoxin. Needles (Me_2CO). Mp 255-256°. $[\alpha]_D^{24}$ +37 (c, 0.08 in Me_2CO). λ_{max} 212 (ϵ 26700); 240 (sh) (ϵ 8600); 283 (ϵ 15400); 330 (ϵ 1000) (MeOH).

Sassa, T. *et al., Biosci., Biotechnol., Biochem.*, 2004, **68**, 2633-2636 (*isol, pmr, cmr*)

Acridone **A-112**

9(10H)-Acridinone, 9CI. 9-Hydroxyacridine. 9-Acridinol. Acridol
[578-95-0]



NH-*form* OH-*form*

$C_{13}H_9NO$ 195.22
NH-form predominates. Constit. of the roots and rhizomes of *Thamnosma montana* (Rutaceae). Antineoplastic agent. Yellow leaflets (EtOH). Insol. Et_2O, C_6H_6, $CHCl_3$. Mp 356-358° Mp 362-365° dec. pK_{a1} -0.32 (20°, H_2SO_4 aq.).
▸AR6976000

NH-form

N-*Benzoyl: 10-Benzoyl-9(10*H*)-acridinone, 9CI*
[57479-66-0]
$C_{20}H_{13}NO_2$ 299.328
Yellow plates (hexane or by subl.). Mp 198-200°.

N-*Me:* see 10-Methylacridone, M-382

N-*Et: 10-Ethylacridone*
[2207-41-2]
$C_{15}H_{13}NO$ 223.274
Mp 159°.

OH-form [643-62-9]

Me ether: 9-Methoxyacridine
[10228-90-7]
$C_{14}H_{11}NO$ 209.247
Yellow needles (petrol). Mp 65°. pK_a 7 (20°). Forms monohydrate with Mp 103°.

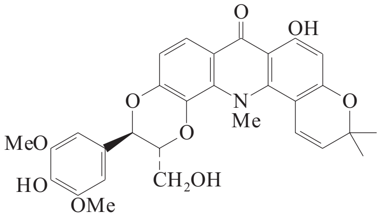
Et ether: 9-Ethoxyacridine
$C_{15}H_{13}NO$ 223.274
Anal. reagent for 1-Hydrazinophthalazine and 4-Amino-3-isoxazolidinone, A-832. Mp *ca.* 83° Mp 92°.

Ph ether: 9-Phenoxyacridine
[2148-14-3]
$C_{19}H_{13}NO$ 271.318
Cryst. (C_6H_6). Mp 127-128°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 922B (*nmr*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 904B (*ir*)
Kliegl, A. *et al., Ber.*, 1914, **47**, 1629-1640 (*synth*)
Lehmstedt, K. *et al., Ber.*, 1935, **68**, 1455-1464 (*synth, Me ether*)
Org. Synth., Coll. Vol., 2, 1943, 15 (*synth*)
Dupré, D.J. *et al., J.C.S.*, 1945, 549-551 (*Ph ether, synth*)
Kitani, K. *et al., Nippon Kagaku Kaishi*, 1954, **75**, 396-398; *CA*, **49**, 10297 (*Me ether, Et ether, synth*)
Albert, A. *et al., The Acridines*, 2nd edn., E. Arnold, London, 1966, (*rev*)
Altiparmakian, R.H. *et al., Helv. Chim. Acta*, 1972, **55**, 85 (*pmr*)
Gagan, J.M.F. *et al., Acridines*, (Ed. Acheson, R.M.), 2nd edn., Interscience, N.Y., 1973, 141 (*rev*)
Chen, G.J. *et al., J.C.S. Perkin 1*, 1975, 1138 (*synth, N-benzoyl*)
Chang, P.T.O. *et al., J. Nat. Prod.*, 1976, **39**, 134 (*isol, uv, ir, pmr, ms*)
Beak, P. *et al., J.A.C.S.*, 1976, **98**, 171 (*uv*)
Adams, J.H. *et al., J.C.S. Perkin 1*, 1977, 2173 (*synth*)
Faure, R. *et al., Spectrosc. Lett.*, 1981, **14**, 223 (*cmr*)
Stewart, J.T. *et al., Int. J. Pharm.*, 1983, **17**, 161-166 (*Me ether, synth, use*)
Stewart, J.T. *et al., J. Pharm. Sci.*, 1988, **77**, 452-454 (*Me ether, synth, use*)
Potts, G.D. *et al., Acta Cryst. C*, 1995, **51**, 267 (*cryst struct*)
Phanstiel, O. *et al., J.O.C.*, 2000, **65**, 5590-5599 (*Ph ether, synth, pmr*)
Dadabhoy, A. *et al., J.C.S. Perkin 2*, 2002, 348-357 (*N-Et, synth, ir, uv, pmr, cmr*)
Ebead, Y. *et al., Acta Cryst. C*, 2005, **61**, o85-o87 (*Ph ether, cryst struct*)

Acrignine A **A-113**

[149155-25-9]



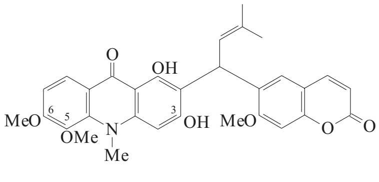
$C_{30}H_{29}NO_9$ 547.56

Acridone-lignan hybrid. Alkaloid from roots of *Citrus grandis* f. Hirado and *Citrus yuko* (Rutaceae). Yellow prisms. Mp 177-179°. Racemic.

Takemura, Y. *et al., Chem. Pharm. Bull.*, 1993, **41**, 406 (*isol, uv, ir, pmr, cmr, cryst struct*)

Acrimarine A **A-114**

[119152-47-5]



$C_{31}H_{29}NO_8$ 543.572
Alkaloid from the roots of *Citrus funadoko* (Rutaceae). Pale yellow oil. $[\alpha]_D$ -9.76 (c, 0.082 in $CHCl_3$).

3-Me ether: ***Acrimarine N***
$C_{32}H_{31}NO_8$ 557.599
Alkaloid from roots of Yalaha [several hybrid seedlings resulting from a cross of Duncan grapefruit (*Citrus paradisi*) x Dancy tangerine (*Citrus tangerina*)].

Yellow oil. Opt. inactive.

3-Me ether, N*-de-Me:* ***Acrimarine B***
[119152-48-6]
$C_{31}H_{29}NO_8$ 543.572
Alkaloid from the roots of *Citrus funadoko* (Rutaceae). Yellow prisms (Me_2CO). Mp 288-290°. $[\alpha]_D$ -7.14 (c, 0.056 in $CHCl_3$).

O^6*-De-Me:* ***Acrimarine K***
[147395-91-3]
$C_{30}H_{27}NO_8$ 529.545
Alkaloid from roots of *Citrus funadoko* (Rutaceae). Yellow oil. $[\alpha]_D^{25}$ 0 (c, 0.0695 in $CHCl_3$).

O^6*-De-Me, 3-Me ether:* ***Acrimarine F***
[129722-89-0]
$C_{31}H_{29}NO_8$ 543.572
Alkaloid from the roots of *Citrus funadoko* (Rutaceae). Pale yellow powder.

O^6*-De-Me, 3-Me ether,* N^6*-de-Me:* ***Acrimarine E***
[129722-88-9]
$C_{30}H_{27}NO_8$ 529.545
Alkaloid from the roots of *Citrus funadoko* (Rutaceae). Pale yellow prisms (Me_2CO). Mp 274-276°. $[\alpha]_D$ +20.1 (c, 0.05 in Me_2CO).

6-Demethoxy, O^5*-de-Me:* ***Acrimarine G***
[129722-97-0]
$C_{29}H_{25}NO_7$ 499.519
Alkaloid from the roots of *Citrus funadoko* (Rutaceae). Yellow oil. $[\alpha]_D$ +8 (c, 0.075 in $CHCl_3$).

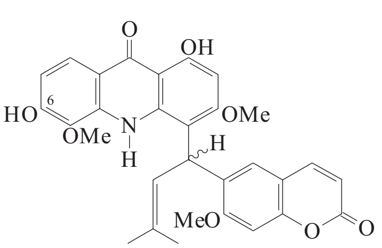
6-Demethoxy, O^5*-de-Me, 3-Me ether:* ***Acrimarine H***
[132185-44-5]
$C_{30}H_{27}NO_7$ 513.546
Alkaloid from roots of *Citrus* spp. Yellow oil. $[\alpha]_D$ 0 (Me_2CO).

Bis(demethoxy): ***Acrimarine M***
[147513-68-6]
$C_{29}H_{25}NO_6$ 483.52
Alkaloid from roots of *Citrus funadoko* (Rutaceae). Yellow oil. $[\alpha]_D^{25}$ 0 (c, 0.052 in $CHCl_3$).

Ito, C. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2586 (*Acrimarine H*)
Furukawa, H. *et al., J.C.S. Perkin 1*, 1990, 1593 (*isol, pmr, cmr, struct*)
Takemura, Y. *et al., Heterocycles*, 1992, **34**, 2363 (*Acrimarine K, Acrimarine M*)
Takemura, Y. *et al., Heterocycles*, 1994, **38**, 1937 (*Acrimarine N*)

Acrimarine C A-115

[119206-24-5]



$C_{30}H_{27}NO_8$ 529.545

(-)-form
Alkaloid from the roots of *Citrus funadoko* (Rutaceae). Yellow oil. $[\alpha]_D$ -6.17 (c, 0.081 in $CHCl_3$).

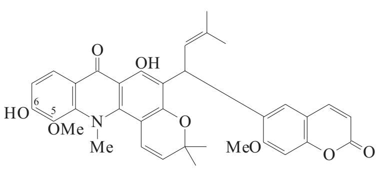
6-Me ether: ***Acrimarine D***
[129722-87-8]
$C_{31}H_{29}NO_8$ 543.572
Alkaloid from the root of *Citrus funadoko* (Rutaceae). Yellow oil. $[\alpha]_D$ -3 (c, 0.103 in $CHCl_3$).

(±)-form
Acrimarine L
[147512-44-5]
From roots of *Citrus funadoko* (Rutaceae). Yellow oil.

Furukawa, H. *et al., J.C.S. Perkin 1*, 1990, 1593 (*Acrimarine C, Acrimarine D*)
Takemura, Y. *et al., Heterocycles*, 1992, **34**, 2363 (*Acrimarine L*)

Acrimarine J A-116

[147395-90-2]



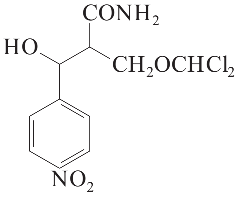
$C_{35}H_{33}NO_8$ 595.648
Alkaloid from roots of Yalaha [several hybrid seedlings resulting from a cross of Duncan grapefruit (*Citrus paradisii*) × Dancy tangerine (*Citrus tangerina*)] (Rutaceae). Yellow oil. $[\alpha]_D^{28}$ 0 (c, 0.106 in $CHCl_3$).

6-Deoxy, O^5*-de-Me:* ***Acrimarine I***
[147395-89-9]
$C_{34}H_{31}NO_7$ 565.621
Alkaloid from roots of Yalaha (Rutaceae). Yellow oil. $[\alpha]_D^{26}$ +27.8 (c, 0.036 in $CHCl_3$).

Takemura, Y. *et al., Heterocycles*, 1992, **34**, 2363 (*isol, uv, ir, pmr, cmr, ms, struct*)

Acrodontiolamide A-117

α-(Dichloromethoxymethyl)-β-hydroxy-4-nitrobenzenepropanamide
[152053-09-3]

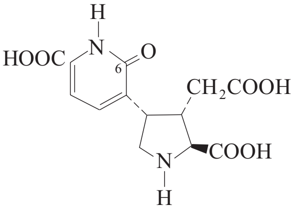


$C_{11}H_{12}Cl_2N_2O_5$ 323.132
Metab. of the fungus *Acrodontium salmoneum*. Antifungal agent. Plates (MeOH). Mp 145-147°. λ_{max} 273 (ϵ 386000) (MeOH) (Berdy).

Buarque de Gusmao, N. *et al., Spectrosc. Lett.*, 1993, **26**, 1373 (*isol, uv, ir, ms, pmr, cmr*)
Steiman, R. *et al., Pharmazie*, 1995, **50**, 693 (*isol, activity*)

Acromelic acid A A-118

5-[5-Carboxy-4-(carboxymethyl)-3-pyrrolidinyl]-1,6-dihydro-6-oxo-2-pyridinecarboxylic acid, 9CI. Acromelinic acid A
[86630-09-3]



$C_{13}H_{14}N_2O_7$ 310.263
Trace alkaloid from fruiting bodies of the poisonous mushroom *Clitocybe acromelalga*. Shows very potent neuroexcitatory action. Cryst. Sol. H_2O; poorly sol. Me_2CO, hexane. Mp 310°. $[\alpha]_D$ +27.8 (c, 0.35 in H_2O). Struct. established by synth. Phys. props. are of synthetic material. λ_{max} 240 (ϵ 4370); 315 (ϵ 8910) (pH 2) (Derep). λ_{max} 241 (ϵ 5130); 312 (ϵ 9120) (pH 12) (Derep). λ_{max} 243 (ϵ 5500); 315 (ϵ 9550) (H_2O pH 7) (Derep). λ_{max} 242 ; 317 (pH 7 buffer) (Berdy). λ_{max} 240 ; 313 (pH 2 buffer) (Berdy). λ_{max} 241 ; 312 (pH 12 buffer) (Berdy). λ_{max} 240 (ϵ 5130); 313 (ϵ 9550) (H_2O) (Berdy).

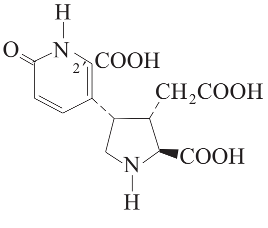
6-Deoxo, 5,6-didehydro: ***Acromelic acid D***
[102329-71-5]
$C_{13}H_{14}N_2O_6$ 294.263
Minor constit. of the toxic mushroom *Clitocybe acromelalga*. Sol. H_2O. $[\alpha]_D$ +17.6 (c, 0.07 in H_2O). λ_{max} 221 ; 269 (H_2O) (Berdy).

6-Deoxo, 5,6-didehydro, 4-decarboxy, 6-carboxy: Acromelic acid E
[145237-01-0]
$C_{13}H_{14}N_2O_6$ 294.263
Minor constit. of the toxic mushroom *Clitocybe acromelalga*. Sol. H_2O. λ_{max} 266 (H_2O) (Berdy).

Takano, S. *et al., J.A.C.S.*, 1987, **109**, 5523 (*synth*)
Konno, K. *et al., J.A.C.S.*, 1988, **110**, 4807; 6926 (*isol, synth, ir, uv, pmr*)
Takano, S. *et al., Heterocycles*, 1989, **29**, 1473 (*synth, bibl*)
Fushiya, S. *et al., Heterocycles*, 1992, **34**, 1277 (*isol, pmr, cd, struct*)
Barco, A. *et al., Gazz. Chim. Ital.*, 1993, **123**, 185 (*synth*)
Baldwin, J.E. *et al., Tetrahedron*, 1998, **54**, 7465-7484 (*synth*)

Acromelic acid B A-119

3-[5-Carboxy-4-(carboxymethyl)-3-pyrrolidinyl]-1,6-dihydro-6-oxo-2-pyridinecarboxylic acid, 9CI. Acromelinic acid B
[86630-10-6]



$C_{13}H_{14}N_2O_7$ 310.263
Trace alkaloid from the poisonous mushroom *Clitocybe acromelalga*. Shows very potent neuroexcitatory action. Amorph. powder. Sol. H_2O; poorly sol. Me_2CO, hexane. $[\alpha]_D$ +50.1 (c, 0.45 in H_2O). Struct. established by synth. Phys. props. are of synthetic material. λ_{max} 231; 308 (pH 2) (Derep). λ_{max} 241; 311 (pH 12) (Derep). λ_{max} 227; 300 (pH 7) (Derep). λ_{max} 236 (ϵ 6320); 302 (ϵ 2920) (MeOH) (Berdy).

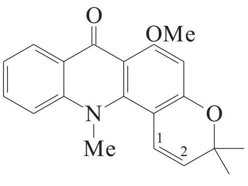
2′-Decarboxy: ***Acromelic acid C***
[133740-47-3]
$C_{12}H_{14}N_2O_5$ 266.253
From *Clitocybe acromelalga*. Powder. $[\alpha]_D$ +31.9 (c, 0.23 in H_2O). λ_{max} 230 (ϵ 11000); 302 (ϵ 6150) (MeOH) (Derep). λ_{max} 230 (ϵ 10592); 301 (ϵ 6150) (H_2O) (Berdy).

▶ LD_{50} (mus, ipr) 10 mg/kg.

Hashimoto, K. *et al., Chem. Lett.*, 1986, 1399 (*synth, uv, ir, cd, abs config*)
Konno, K. *et al., J.A.C.S.*, 1988, **110**, 4807; 6926 (*isol, uv, pmr, synth, struct*)
Takano, S. *et al., Heterocycles*, 1989, **29**, 1473 (*synth, bibl*)
Fushiya, S. *et al., Tet. Lett.*, 1990, **31**, 3901 (*Acromelic acid C*)

Acronycine A-120

*3,12-Dihydro-6-methoxy-3,3,12-trimethyl-7*H*-pyrano[2,3-*c*]acridin-7-one, 9CI, 8CI.*
Acronine, INN, USAN*. NSC 403169. Compound 42339*
[7008-42-6]



$C_{20}H_{19}NO_3$ 321.375
Alkaloid from *Acronychia baueri* (*Bauerella baueri*), *Melicope leptococca* and *Sarcomelicope argyrophylla*. Antineoplastic agent. . Yellow needles (EtOH). Mp 175-176°. Log P 3.7 (calc). λ_{max} 280 (ϵ 39800); 291 (ϵ 34700); 304 (ϵ 19100); 392 (ϵ 6920) (EtOH) (Derep). λ_{max} 224 (ϵ 24500); 281 (ϵ 48000); 293 (ϵ 43500); 308 (ϵ 40700); 380 (ϵ 10250) (MeOH) (Berdy).

▶ LD_{50} (mus, orl) 522 mg/kg. Exp. carcinogenic data. UQ0330000

Hydrochloride: [70509-95-4]
Red needles (H_2O). Mp 125-130°. Heating above melting point causes *O*-demethylation.

N*-De-Me:* ***De-*N*-methylacronycine****. Des-*N*-methylacronycine*
[13255-08-8]
$C_{19}H_{17}NO_3$ 307.348
Alkaloid from *Glycosmis pentaphylla* and *Murraya paniculata* (Rutaceae). Yellow needles (Me_2CO). Mp 268-270° dec. (with sintering at 260°). λ_{max} 280 (ϵ 39800); 291 (ϵ 34700); 304 (ϵ 19100); 392 (ϵ 6920) (EtOH) (Derep).

N*-De-Me, hydrochloride:*
Orange-red needles ($MeOH/Et_2O$). Mp 137-141°.

N*-De-Me, picrate:*
Orange needles (EtOH). Mp 222-224° dec.

O*-De-Me:* ***Noracronycine****. Noracronine*
[13161-79-0]
$C_{19}H_{17}NO_3$ 307.348
Alkaloid from *Glycosmis pentaphylla*, *Murraya paniculata* and *Boenninghausenia albiflora*. Bright yellow needles (C_6H_6 or EtOAc). Mp 203-205°.

O*-De-Me, Ac:*
Yellow rods (EtOAc). Mp 201-203°.

O,N*-Di-de-Me:* ***De-*N*-methylnoracronycine****. Des-*N*-methylnoracronycine*
[13396-93-5]
$C_{18}H_{15}NO_3$ 293.321
Alkaloid from *Glycosmis pentaphylla* (Rutaceae). Has antitumour activity. Bright yellow needles (C_6H_6/EtOAc). Mp 245-246°.

▶ Carcinogenic.

O,N*-Di-de-Me,* O*-Ac:* [36385-14-5]
Fluffy needles ($CHCl_3$/EtOAc). Mp 235-236.5°.

1,2-Epoxide: ***Acronycine epoxide***
[118964-07-1]
$C_{20}H_{19}NO_4$ 337.374
Alkaloid from the bark of *Sarcomelicope simplicifolia* ssp. *neoscotica*. Pale yellow foam. $[\alpha]_D^{20}$ +2 (c, 0.25 in CH_2Cl_2).

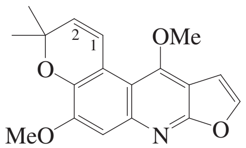
1,2-Dihydro, 1-oxo, 2ξ-hydroxy, O,N*-di-de-Me:* ***1,2-Dihydro-2-hydroxy-*N*-de-methyl-1-oxonoracronycine***
$C_{18}H_{15}NO_5$ 325.32
Alkaloid from the bark of *Medicosma subsessilis*. Amorph. yellow solid. λ_{max} 221 (log ϵ 4.98); 255 (log ϵ 4.99); 383 (log ϵ 4.04) (EtOH).

11-Methoxy, O*-de-Me:* ***5-Methoxynoracronycine****. Baiyumine A*
[51179-68-1]
$C_{20}H_{19}NO_4$ 337.374
Alkaloid from the bark of *Citrus junos* (yuzu) and *Citrus grandis* f. *hakunikuyu* (Rutaceae). Light yellow prisms, or orange needles (Me_2CO/hexane), or orange plates (Et_2O). Mp 146-148° Mp 160-161° (155-157°).

Hughes, G.K. *et al., Nature (London)*, 1948, **162**, 223 (*isol*)
Drummond, L.J. *et al., Aust. J. Sci. Res., Ser. A*, 1949, **2**, 630 (*isol, struct*)
Brown, R.D. *et al., Aust. J. Sci. Res., Ser. A*, 1950, **3**, 593 (*struct*)
MacDonald, P.L. *et al., Aust. J. Chem.*, 1966, **19**, 275 (*struct*)
Svoboda, G.H. *et al., J. Nat. Prod.*, 1966, **29**, 206 (*rev*)
Svoboda, G.H. *et al., J. Pharm. Sci.*, 1966, **55**, 758 (*pharmacol*)
Govindachari, T.R. *et al., Tetrahedron*, 1966, **22**, 3245 (*Noracronycine, De-N-methylacronycine*)
Beck, J.R. *et al., J.A.C.S.*, 1968, **90**, 4706 (*synth*)
Gougoutas, J.Z. *et al., Acta Cryst. B*, 1970, **26**, 853 (*cryst struct*)
Hlubucek, J. *et al., Aust. J. Chem.*, 1970, **23**, 1881 (*synth*)
Sullivan, H.R. *et al., J. Med. Chem.*, 1970, **13**, 904 (*metab*)
Gout, P.W. *et al., J. Cell Physiol.*, 1972, **78**, 127 (*biochem*)
Schneider, J. *et al., J. Med. Chem.*, 1972, **15**, 266 (*synth, tox, derivs*)
Lahey, F.M. *et al., Aust. J. Chem.*, 1973, **26**, 2311 (*synth*)
Tan, P. *et al., Cancer Res.*, 1973, **33**, 2320 (*pharmacol*)
Saxton, J.E. *et al., Chem. Heterocycl. Compd.*, 1973, **9**, 379 (*rev*)
Betts, R.E. *et al., J. Med. Chem.*, 1974, **17**, 599
Brannon, D.R. *et al., J. Med. Chem.*, 1974, **17**, 653
Bandranayake, W. *et al., J.C.S. Perkin 1*, 1974, 998 (*synth*)
Bert, M. *et al., Phytochemistry*, 1974, **13**, 301 (*isol*)
Blechert, S. *et al., Chem. Ber.*, 1978, **111**, 439 (*synth*)
Rózsa, Zs. *et al., Phytochemistry*, 1978, **17**, 169 (*isol, uv, ir, derivs*)
Adams, J.H. *et al., Tetrahedron*, 1981, **37**, 209 (*synth*)
Gerzon, K. *et al., Alkaloids (Academic Press)*, 1983, **21**, 1 (*rev*)
Funayama, S. *et al., J. Nat. Prod.*, 1983, **46**, 391 (*cmr*)
Skaltsounis, A.L. *et al., J. Nat. Prod.*, 1983, **46**, 732 (*isol*)
Reisch, J. *et al., Annalen*, 1984, 31 (*synth*)
Watanabe, M. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1264 (*synth, bibl*)
Funayama, S. *et al., Planta Med.*, 1984, **50**, 121 (*pmr*)
Brum-Bousquet, M. *et al., Planta Med.*, 1985, **51**, 536; 1988, **54**, 470 (*isol, uv, ir, pmr, ms, struct, epoxide*)
Ju-ichi, M. *et al., Heterocycles*, 1986, **24**, 1595 (*5-Methoxynoracronycine*)
Wu, T.S. *et al., Phytochemistry*, 1987, **26**, 871 (*Baiyumine A*)
Anand, R.C. *et al., Heterocycles*, 1990, **31**, 1733 (*synth*)
Loughhead, D.G. *et al., J.O.C.*, 1990, **55**, 2245 (*synth, Acronycine, Des-N-methylacronycine*)
Horne, S. *et al., Chem. Comm.*, 1991, 1046 (*synth*)
Reisch, J. *et al., Annalen*, 1994, 317 (*synth, Acronycine epoxide*)
Anand, R.C. *et al., Chem. Comm.*, 1996, 199 (*synth, Acronycine, Des-N-methylacronycine*)
Tillequin, F. *et al., Alkaloids: Chem. Biol. Perspect.*, 1998, **12**, 1-102 (*rev*)
Minh, N.T. *et al., Z. Naturforsch., B*, 2003, **58**, 1234-1236 (*Dihydrohydroxydemethyloxonoracronycine*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADR750

Acronydine A-121

*5,11-Dimethoxy-3,3-dimethyl-3*H*-furano[2,3-*b*]pyrano[3,2-*f*]quinoline, 9CI*
[518-68-3]



$C_{18}H_{17}NO_4$ 311.337
Alkaloid from *Acronychia baueri, Melicope leptococca* and *Sarcomelicope leiocarpa* (Rutaceae). Prisms (MeOH). Mp 151-153°.

Picrate:

Yellow needles (propanol or EtOH). Mp 216-218° dec.

*1,2-Dihydro, 1*R*,2*R*-dihydroxy:* **cis-*1,2-Dihydro-1,2-dihydroxyacronydine*.** cis-*1,2-Dihydroxy-1,2-dihydroacronydine*
[126661-84-5]
$C_{18}H_{19}NO_6$ 345.351
Alkaloid from bark of *Sarcomelicope dogniensis*. Noncryst. $[\alpha]_D$ +2 (c, 0.25 in MeOH). λ_{max} 225 (sh) (log ϵ 4.17); 254 (log ϵ 4.43); 303 (sh) (log ϵ 3.88); 317 (log ϵ 4.05); 329 (log ϵ 4.04); 344 (sh) (log ϵ 3.83) (MeOH).

*1,2-Dihydro, 1*R*,2*S*-dihydroxy:* **trans-*1,2-Dihydro-1,2-dihydroxyacronydine*.** trans-*1,2-Dihydroxy-1,2-dihydroacronydine*
[126661-85-6]
$C_{18}H_{19}NO_6$ 345.351
Alkaloid from bark of *Sarcomelicope dogniensis*. Mp 178-180°. $[\alpha]_D$ -8 (c, 0.2 in MeOH). λ_{max} 225 (sh) ; 254 (log ϵ 4.43); 303 (sh) (log ϵ 3.88); 317 (log ϵ 4.05); 329 (log ϵ 4.04); 344 (sh) (log ϵ 3.83) (MeOH).

*5-Demethoxy: 11-Methoxy-3,3-dimethyl-3*H*-furano[2,3-*b*]pyrano[3,2-*f*]quinoline.* ***Medicosmine***
[35306-86-6]
$C_{17}H_{15}NO_3$ 281.31
Alkaloid from *Boronella koniambiensis* and *Medicosma cunninghamii*. Pale cream needles (EtOH or ETOAc/petrol). Mp 138.5-139.5°.

5-Demethoxy, picrate:
Fine yellow needles (EtOH). Mp 190-191°.

*5-Demethoxy, 1,2-dihydro, 1*R**,2**R*-dihydroxy:* **cis-*1,2-Dihydro-1,2-dihydroxymedicosmine*.** cis-*1,2-Dihydroxy-1,2-dihydromedicosmine*
$C_{17}H_{17}NO_5$ 315.325
Alkaloid from the aerial parts of *Boronella koniambiensis*. Amorph. solid. $[\alpha]_D$ -5 (c, 0.1 in $CHCl_3$). λ_{max} 245 ; 300 ; 312 ; 342 ; 357 (MeOH).

Lamberton, J.A. *et al., Aust. J. Chem.*, 1953, **6**, 66; 173 (*Acronydine, Medicosmine, isol*)
Johns, S.R. *et al., Aust. J. Chem.*, 1967, **20**, 1975, (*pmr, struct*)
Govaindachari, T.R. *et al., Indian J. Biochem.*, 1971, **9**, 1031 (*Medicosmine, synth, uv, pmr*)
Skaltsounis, A.L. *et al., J. Nat. Prod.*, 1983, **46**, 732
Baudouin, G. *et al., J. Nat. Prod.*, 1985, **48**, 260
Mitaku, S. *et al., Ann. Pharm. Fr.*, 1989, **47**, 149-156 (*1,2-Dihydro-1,2-dihydroxyacronydine*)
Grougnet, R. *et al., J. Nat. Prod.*, 2005, **68**, 1083-1086 (*1,2-Dihydro-1,2-dihydroxymedicosmine, Medicosmine*)

Acsine A-122

[1353-77-1]

$C_{21}H_{29}NO_5$ 375.464

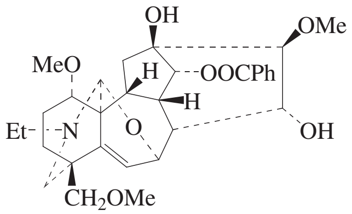
Struct. unknown. Alkaloid from the roots of *Aconitum excelsum* (Ranunculaceae). Mp 182-185° (slow heating) Mp 192-195° (rapid heating). Contains OAc and 2 OH groups, plus an ether linkage.

Sulfate: Mp 220° dec.

Platonova, T.F. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1958, **28**, 259 (*isol, ir*)

Acsonine A-123

[367452-76-4]



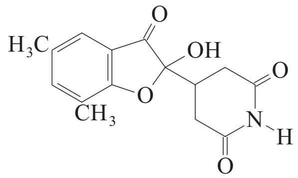
$C_{31}H_{41}NO_8$ 555.667

Unusual 7,17-epoxyaconitane struct. Alkaloid from the roots of *Aconitum kusnezoffii*. Amorph. powder.

Zinurova, E.G. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2001, **50**, 311-312 (*isol, pmr, cmr*)

Actiketal A-124

4-(2,3-Dihydro-2-hydroxy-5,7-dimethyl-3-oxo-2-benzofuranyl)-2,6-piperidinedione, 9CI. RK 4415. Antibiotic RK 4415
[133658-47-6]

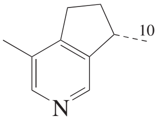


$C_{15}H_{15}NO_5$ 289.287

Glutarimide-type antibiotic. Prod. by *Streptomyces pulveraceus* ssp. *epiderstagenes*. Antitumour agent. Powder. Mp 96-100°. $[\alpha]_D$ 0. λ_{max} 222 (ϵ 9710); 264 (ϵ 7630); 350 (ϵ 2490) (MeOH) (Derep).

Sonoda, T. *et al., J. Antibiot.*, 1991, **44**, 160 (*isol, pmr, cmr*)
Japan. Pat., 1991, 91 255 082; *CA*, **116**, 126985g (*isol*)
Kiyota, H. *et al., Tet. Lett.*, 2000, **41**, 5887-5890 (*synth*)

Actinidine A-125



(*S*)*-form*

$C_{10}H_{13}N$ 147.219

(*R*)*-form* [15524-81-9]
Synthetic. Liq. Bp_{10} 92-94°. $[\alpha]_D^{20}$ +10.8 (c, 0.36 in $CHCl_3$).
Picrate: Mp 146-147°.

(*S*)*-form* [524-03-8]
Alkaloid from *Actinidia arguta* (taravine), *Actinidia polygama, Tecoma fulva, Tecoma radicans* and *Valeriana officinalis* (valerian). Constit. of defensive secretions of various insects incl. *Megacrania alpheus*, *Ontholestes murinus* and *Tapinoma erraticum*). Powerful attractant for Felidae (cats). Oil. Bp_9 100-103°. $[\alpha]_D^{11}$ -7.2 ($CHCl_3$).
Picrate: Mp 143°.

N-*[2-(4-Hydroxyphenyl)ethyl]:* **N-*(*p*-Hydroxyphenethyl)actinidine***
[15794-92-0]
$C_{18}H_{22}NO^{\oplus}$ 268.378
Quaternary alkaloid from the roots of *Valeriana officinalis* (valerian). Mp 201-203° dec. (as chloride). $[\alpha]_D^{22}$ +50.5 (MeOH).

10-Acetoxy: ***10-Acetoxyactinidine***
$C_{12}H_{15}NO_2$ 205.256
Alkaloid from the roots of *Argylia radiata*. Amorph. solid. Stereochem. not certain.

(±)*-form* [79254-93-6]
Synthetic. Oil. Mp 146-146.5° (as picrate). Bp_9 100-103°.

Sakan, T. *et al., Bull. Chem. Soc. Jpn.*, 1959, **32**, 315; 1155; 1960, **33**, 712 (*uv, ir, isol, struct, synth*)
Djerassi, C. *et al., Chem. Ind. (London)*, 1961, 210 (*pmr*)
Torssell, K. *et al., Acta Chem. Scand.*, 1967, **21**, 53 (*N-4-Hydroxyphenethylactinidine*)
Cavill, G.W.K. *et al., Aust. J. Chem.*, 1967, **20**, 349 (*synth, uv, pmr*)
Johnson, R.D. *et al., Phytochemistry*, 1971, **10**, 3334 (*isol, ms*)
Wuest, J.D. *et al., J.O.C.*, 1977, **42**, 2111 (*synth*)
Nitta, M. *et al., Chem. Lett.*, 1981, 933 (*synth*)
Davies, L.B. *et al., J.C.S. Perkin 1*, 1981, 1909 (*synth, uv, ir, pmr, ms*)
Tomalski, M.D. *et al., J. Chem. Ecol.*, 1987, **13**, 253-263 (*isol, ms*)
Cossy, J. *et al., Tet. Lett.*, 1988, **29**, 6113 (*synth*)
Ranarivelo, Y. *et al., Heterocycles*, 1990, **31**, 1727-1731 (*(S)-form, synth*)
Huth, A. *et al., J. Chem. Ecol.*, 1990, **16**, 2691-2711 (*isol*)
Cossy, J. *et al., J.O.C.*, 1993, **58**, 2351 (*synth*)
Shiao, M.J. *et al., J.O.C.*, 1993, **58**, 3162 (*synth*)
Stepanov, A.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1998, **47**, 2286-2291 (*synth*)
Jones, K. *et al., Tetrahedron*, 1998, **54**, 2275-2280 (*synth*)
Bianco, A. *et al., Nat. Prod. Lett.*, 2002, **16**, 77-80 (*10-Acetoxyactinidine*)

Actinine A-126

*3-Carboxy-*N,N,N*-trimethyl-1-propanaminium hydroxide inner salt, 9CI. Tri-*N*-methyl-γ-butyrobetaine. 4-Aminobutanoic acid betaine. γ-Butyrobetaine. Butyrobetaine. 4-Aminobutanoic acid trimethylbetaine*
[407-64-7]
$Me_3N^{\oplus}CH_2CH_2CH_2COO^{\ominus}$

$C_7H_{15}NO_2$ 145.201

Inner salt. Occurs in the sea-rose *Actinia equina*, in muscles of various snakes and in urine in cases of pernicious anaemia. Isol. from brain tissue. Also from *Polyporus sulphureus*. Biosynthetic intermed. in synth. of Carnitine. Plates + $3H_2O$ (EtOH/Et_2O aq.). Sol. EtOH. Dec. at 220°.

▶ BP3930000

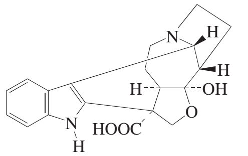
Hydrochloride: [6249-56-5]
Mp 203° Mp 214-219°.

▶ BP3850000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 681A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 878B (*nmr*)
Engeland, R. *et al., Ber.*, 1921, **54**, 2212 (*derivs*)
Linneweh, W. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1928, **175**, 95; **176**, 220; 1929, **181**, 48; **182**, 9 (*isol*)
List, P.H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1959, **292**, 260 (*isol*)
Hosein, E.A. *et al., Nature (London)*, 1960, **187**, 321 (*isol*)
Cox, R.A. *et al., Biochem. J.*, 1973, **136**, 1083 (*biosynth*)
Anderson, L. *et al., Synthesis*, 1981, 468 (*synth*)

Actinophyllic acid A-127

[845959-90-2]



Absolute Configuration

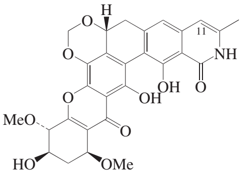
$C_{19}H_{20}N_2O_4$ 340.378

Indole alkaloid of unknown biogenetic relationships. Alkaloid from the leaves of *Alstonia actinophylla*. Inhibitor of Carboxypeptidase U/Hippuricase. Brown gum. $[\alpha]_D$ -29 (c, 0.001 in MeOH). λ_{max} 217 (ε 24410); 280 (ε 17000) (MeOH).

Carroll, A.R. *et al., J.O.C.*, 2005, **70**, 1096-1099 (*isol, biosynth, pmr, cmr*)
Martin, C.L. *et al., J.A.C.S.*, 2008, **130**, 7568-7569 (*synth*)

Actinoplanone D A-128

*3,4,8a,13-Tetrahydro-3,15,16-trihydroxy-1,4-dimethoxy-12-methyl-1*H*-xantheno[4′,3′,2′:4,5][1,3]benzodioxino[7,6-g]isoquinoline-14,17(2*H*,9*H*)-dione, 9CI*
[116200-81-8]



Absolute Configuration

$C_{28}H_{25}NO_{10}$ 535.506

CAS numbering shown. Isol. from *Actinoplanes* sp. R-304. Cytotoxic agent. Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 222-224° dec. $[\alpha]_D^{25}$ -624.1 (c, 0.7 in $CHCl_3$). λ_{max} 221 (ε 20900); 249 (ε 24500); 298 (ε 12000); 312 (ε 11220); 328 (ε 10960); 358 (ε 16200); 372 (ε 17400) (EtOH) (Derep).

N-*Amino:* ***Actinoplanone C***
[116200-80-7]
$C_{28}H_{26}N_2O_{10}$ 550.521
Isol. from *Actinoplanes* sp. R-304. Cytotoxic agent. Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 278-280° dec. $[\alpha]_D^{25}$ -646.1 (c, 0.35 in $CHCl_3$). λ_{max} 228 (ε 19100); 253 (ε 20400); 302 (ε 14100); 336 (sh) ; 360 (ε 14100); 375 (ε 15500) (EtOH) (Derep).

N-*(3-Oxo-2-butenylideneamino):* ***Actinoplanone G***
[116200-82-9]
$C_{32}H_{30}N_2O_{11}$ 618.596
Isol. from *Actinoplanes* sp. R-304. Cytotoxic agent. Yellowish solid. Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 173-176°. $[\alpha]_D^{25}$ -582.3 (c, 0.44 in $CHCl_3$). λ_{max} 227 (ε 30900); 253 (ε 31600); 304 (ε 14500); 340 (ε 12600); 380 (ε 16600) (EtOH) (Derep).

11-Chloro: ***Actinoplanone B***
[115655-87-3]
$C_{28}H_{24}ClNO_{10}$ 569.951
Isol. from *Actinoplanes* sp. R-304. Cytotoxic agent. Yellow amorph. solid. Sol. MeOH, EtOAc, bases, $CHCl_3$; poorly sol. H_2O. Mp 240-243°. $[\alpha]_D^{25}$ -649.4 (c, 1.54 in $CHCl_3$). λ_{max} 228 (ε 30900); 253 (ε 33100); 305 (ε 13500); 336 (sh) ; 365 (ε 22900); 380 (ε 25100) (EtOH) (Derep). λ_{max} 226 (ε 25100); 252 (ε 28950); 303 (ε 13180); 363 (ε 17790); 377 (ε 19500) (EtOH) (Berdy).

11-Chloro, N-*amino:* ***Actinoplanone A***
[115655-86-2]
$C_{28}H_{25}ClN_2O_{10}$ 584.966
Isol. from *Actinoplanes* sp. R-304. Cytotoxic agent. Yellow needles (Me_2CO). Sol. $CHCl_3$, bases, MeOH, EtOAc; poorly sol. H_2O. Mp 276-278°. $[\alpha]_D^{25}$ -619.8 (c, 0.29 in $CHCl_3$). λ_{max} 228 (ε 30900); 253 (ε 33100); 305 (ε 13500); 336 (sh); 365 (ε 22900); 380 (ε 25100) (EtOH) (Derep).

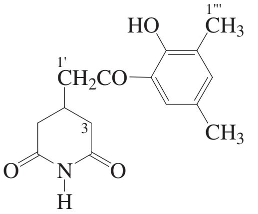
11-Chloro, N-*(isopropylideneamino):* ***Actinoplanone E***
[116229-70-0]
$C_{31}H_{29}ClN_2O_{10}$ 625.03
Isol. from *Actinoplanes* sp. R-304. Cytotoxic agent. Yellowish solid. Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 190-193°. $[\alpha]_D^{25}$ -516.7 (c, 0.21 in $CHCl_3$). λ_{max} 232 (ε 20900); 253 (ε 26300); 308 (ε 10700); 344 (sh); 370 (ε 17400); 386 (ε 18200) (EtOH) (Derep).

11-Chloro, N-*(3-oxo-2-butenylideneamino):* ***Actinoplanone F***
[116200-79-4]
$C_{32}H_{29}ClN_2O_{11}$ 653.041
Isol. from *Actinoplanes* sp. R-304. Cytotoxic agent. Yellowish solid. Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 281-282° dec. λ_{max} 232 (ε 20900); 253 (ε 26300); 308 (ε 10700); 344 (sh); 370 (ε 17400); 386 (ε 18200) (EtOH) (Derep). λ_{max} 231 (ε 31500); 254 (ε 33700); 308 (ε 13800); 386 (ε 18200) (EtOH) (Berdy).

Kobayashi, K. *et al., J. Antibiot.*, 1988, **41**, 502-511 (*Actinoplanones A,B*)
Kobayashi, K. *et al., J. Antibiot.*, 1988, **41**, 741-750 (*Actinoplanones C-G*)

Actiphenol A-129

4-[2-(2-Hydroxy-3,5-dimethylphenyl)-2-oxoethyl]-2,6-piperidinedione, 9CI. 3-(2-Hydroxy-3,5-dimethylphenacyl)glutarimide, 8CI. C 73. Antibiotic C 73
[526-02-3]



$C_{15}H_{17}NO_4$ 275.304

Prod. by *Streptomyces noursei, Streptomyces albulus, Streptomyces griseus* and *Streptomyces pulveraceus*. Fungicide and shows antitumour props. Needles ($MeOH/CH_2Cl_2$). Mp 201-203°.

*3-Hydroxy (3,4-*trans*-):* ***Antibiotic C 73X****. C 73X*
[20988-33-4]
$C_{15}H_{17}NO_5$ 291.303
Prod. by *Streptomyces griseus*. Cryst. λ_{max} 262 (ε 11700); 347 (ε 4300) (MeOH).

▶ LD_{50} (mus, ipr) 100 - 200 mg/kg.

1′-Hydroxy: ***Nong-kang 101G***
[75314-78-2]
$C_{15}H_{17}NO_5$ 291.303
Isol. from *Streptomyces aureus*. λ_{max} 267 (ε 11620); 356 (ε 3820) (EtOH) (Berdy).

1′′′-Hydroxy: ***Antibiotic AH 135Y****. AH 135Y*
[145066-21-3]
$C_{15}H_{17}NO_5$ 291.303
Prod. by *Streptomyces albovinaceus*. Antiherpetic agent. Powder. Sol. MeOH, Me_2CO, DMSO, EtOH, EtOAc; fairly sol. $CHCl_3$, C_6H_6; poorly sol. H_2O, Et_2O, hexane. Mp 220°. λ_{max} 219 (sh) (ε 14800); 260 (ε 7070); 342 (ε 3260) (MeOH/HCl) (Derep). λ_{max} 219 (sh) (ε 18500); 260 (ε 9070); 343 (ε 4030) (MeOH) (Derep). λ_{max} 219 (ε 15472); 260 (ε 9066); 343 (ε 4026) (MeOH) (Berdy). λ_{max} 219 (ε 14921); 260 (ε 7066); 342 (ε 3257) (MeOH-HCl) (Berdy).

Highet, R.J. *et al., Helv. Chim. Acta*, 1959, **42**, 1523 (*isol, struct*)
Rao, K.V. *et al., J.O.C.*, 1960, **25**, 661 (*isol*)
Johnson, F. *et al., J.O.C.*, 1962, **27**, 3658 (*synth*)
Kharatyan, S. *et al., Chem. Ind. (London)*, 1963, 1038 (*biosynth*)
Vondracek, M. *et al., Chem. Ind. (London)*, 1964, 1686 (*isol, uv*)
Spizek, J. *et al., Folia Microbiol. (Prague)*, 1965, **10**, 263 (*synth*)
Siegel, M.R. *et al., Biochem. Pharmacol.*, 1966, **15**, 1213 (*pharmacol*)
Aszalos, A. *et al., J. Med. Chem.*, 1967, **10**, 281-284 (*C 73X*)
Hua, J.C. *et al., CA*, 1980, **93**, 219277 (*Non-kang 101G*)
Zhang, H. *et al., CA*, 1982, **96**, 118576 (*isol*)
Onan, K.D. *et al., Acta Cryst. C*, 1985, **41**, 428 (*cryst struct*)
Uyeda, M. *et al., J. Antibiot.*, 1992, **45**, 1370 (*Antibiotic AH 135Y*)

Aculeacin B A-130

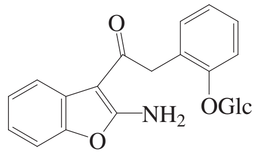
[58814-87-2]

Struct. unknown. Isol. from *Aspergillus aculeatus*. Antibiotic. Amorph. powder. Sol. MeOH, EtOH; fairly sol. EtOAc, H_2O; poorly sol. Me_2CO, hexane, $CHCl_3$. Mp 148-151°. $[\alpha]_D^{24}$ -45 (c, 1 in MeOH). λ_{max} 279 (E1%/1cm 18.5) (MeOH) (Berdy). λ_{max} 247 (E1%/1cm 104); 297 (E1%/1cm 21.6) (MeOH/NaOH) (Berdy).

▶ LD$_{50}$ (mus, ipr) 300 - 900 mg/kg. AU3030000

Japan. Pat., 1976, 76 98 387; *CA*, **86**, 15206w (*isol*)
Satoi, S. *et al., J. Antibiot.*, 1977, **30**, 303-307 (*isol, props*)
Canadian Pat., 1978, 1 041 446; *CA*, **90**, 101942x (*manuf*)

Acuminaminoside A-131



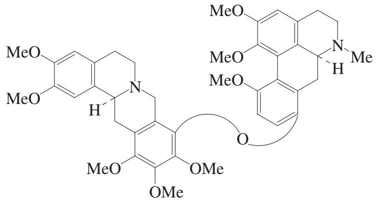
$C_{22}H_{23}NO_8$ 429.426

Constit. of the leaves of *Glochidion acuminatum*. Needles (MeOH). Mp 212-215°. $[\alpha]_D^{28}$ -33.3 (c, 0.75 in MeOH). λ_{max} 214 (log ϵ 4.26); 236 (log ϵ 4); 256 (log ϵ 4.04); 296 (log ϵ 3.99); 310 (log ϵ 4.01) (MeOH).

Otsuka, H. *et al., Chem. Pharm. Bull.*, 2004, **52**, 591-596 (*isol, pmr, cmr, cryst struct*)

Acutiaporberine A-132

[335311-66-5]

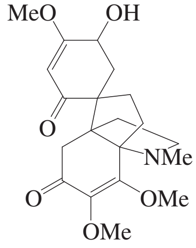


$C_{42}H_{48}N_2O_9$ 724.849

Aporphine-berberine dimer. Alkaloid from the roots of *Thalictrum acutifolium*. Apoptosis-inducing agent. Light yellow flakes. Mp 183.5-184°. $[\alpha]_D^{24}$ -14.2 (c, 3.14 in MeOH).

Chen, Q. *et al., Planta Med.*, 2002, **68**, 550-553 (*isol, activity*)

Acutudaurine A-133



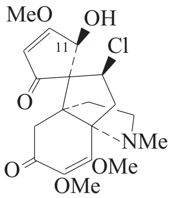
$C_{20}H_{27}NO_6$ 377.436

Stereochem. not determined; but likely to be the same as the related Acutumine, A-134. Alkaloid from the roots of *Menispermum dauricum*. Oil. $[\alpha]_D^{20}$ -102 (c, 0.01 in EtOH). λ_{max} 255 (log ϵ 4.34) (EtOH).

Furumoto, T. *et al., Planta Med.*, 2001, **67**, 194-195

Acutumine A-134

[17088-50-5]



Absolute configuration

$C_{19}H_{24}ClNO_6$ 397.854

Alkaloid from *Sinomenium acutum* and *Menispermum dauricum* (Menispermaceae). Needles. Mp 238-240° dec. $[\alpha]_D^{15}$ -206 (c, 0.69 in Py). pK_a 5.3 (50% EtOH). λ_{max} 245 (ϵ 18970); 270 (ϵ 9750) (EtOH).

Ac:
Needles (Et_2O/hexane). Mp 162-164°. $[\alpha]_D^{20}$ -94 (c, 0.38 in $CHCl_3$).

N-*De-Me:* ***Acutumidine***
[18145-26-1]
$C_{18}H_{22}ClNO_6$ 383.828
Alkaloid from *Sinomenium acutum* and *Menispermum dauricum* (Menispermaceae). Needles. Mp 239-241° dec. $[\alpha]_D^{19}$ -212.5 (c, 0.16 in Py). pK_a 6.6 (50% EtOH). λ_{max} 244 (ϵ 13100); 269 (ϵ 7370) (EtOH).

11-Deoxy: ***Acutuminine***
[23512-32-5]
$C_{19}H_{24}ClNO_5$ 381.855
Alkaloid from the leaves of *Menispermum dauricum* (Menispermaceae). Mp 175-177°. $[\alpha]_D$ -110 ($CHCl_3$). λ_{max} 243 (ϵ 18900); 270 (ϵ 9200) (EtOH).

11-Deoxy, N-*de-Me,* N-*[3-(4-hydroxyphenyl)-2ξ-nitropropyl]:* ***Nitrotyrasacutuminine***
$C_{27}H_{31}ClN_2O_8$ 547.003
Alkaloid from the roots of *Menispermum dauricum*. Powder. $[\alpha]_D^{25}$ -98 (c, 0.2 in MeOH). λ_{max} 251 (log ϵ 3.42); 275 (log ϵ 3.63) (MeOH).

Dechloro: ***Dechloroacutumine***
[219794-33-9]
$C_{19}H_{25}NO_6$ 363.41
Alkaloid from *Menispermum dauricum*. Cryst. (EtOAc/hexane). Mp 178-178.5°. $[\alpha]_D^{25}$ -54 (c, 0.1 in MeOH). λ_{max} 241 (log ϵ 4.27); 268 (log ϵ 3.99) (no solvent reported).

11-Epimer: ***Dauricumine***
[345641-00-1]
$C_{19}H_{24}ClNO_6$ 397.854
Alkaloid from *Menispermum dauricum*. Cryst. (MeOH). Mp 205° dec. $[\alpha]_D^{25}$ -42 (c, 0.1 in Py). λ_{max} 244 (log ϵ 4.16) (MeOH).

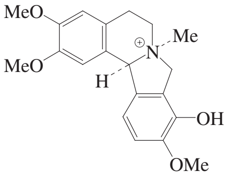
11-Epimer, N-*de-Me:* ***Dauricumidine***
[345640-99-5]
$C_{18}H_{22}ClNO_6$ 383.828
Alkaloid from *Menispermum dauricum*. Powder. Mp 180° dec. $[\alpha]_D^{23}$ +43 (c, 0.1 in Py). λ_{max} 244 (log ϵ 4.11) (MeOH).

11-Epimer, dechloro: ***Dechlorodauricumine***
$C_{19}H_{25}NO_6$ 363.41
Alkaloid from the roots of *Menispermum dauricum*. Amorph. powder. $[\alpha]_D^{25}$ +20.7 (c, 0.1 in MeOH). λ_{max} 242 (log ϵ 4.16) (MeOH).

Nishikawa, M. *et al., J.C.S.(B)*, 1968, 652-658 (*cryst struct, abs config*)
Barton, D.H.R. *et al., J.C.S.(C)*, 1968, 929-936 (*biosynth*)
Okamoto, Y. *et al., Tet. Lett.*, 1969, 1933-1935 (*Acutuminine*)
Tomita, M. *et al., Chem. Pharm. Bull.*, 1971, **19**, 770-791 (*Acutumidine, Acutuminine, Dechloroacutumine*)
Sugimoto, Y. *et al., Phytochemistry*, 1998, **49**, 1293-1297 (*Dechloroacutumine, cryst struct*)
Babiker, H.A.A. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 515-518 (*biosynth, cmr*)
Sugimoto, Y. *et al., J.O.C.*, 2001, **66**, 3299-3302 (*Dauricumidine, Dauricumine*)
Yu, B.-W. *et al., Nat. Prod. Lett.*, 2002, **16**, 155-159 (*Nitrotyrasacutuminine*)
Sugimoto, Y. *et al., Phytochemistry*, 2005, **66**, 2627-2631 (*Dechlorodauricumine*)

Acutupyrrocoline A-135

[163047-26-5]



Absolute Configuration

$C_{20}H_{24}NO_4^{\oplus}$ 342.414

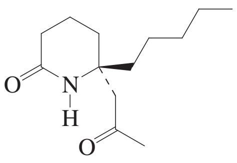
Alkaloid from the rhizomes of *Sinomenium acutum*.

Moriyasu, M. *et al., Nat. Med. (Tokyo)*, 1994, **48**, 287-290

Adalinine A-136

6-(2-Oxopropyl)-6-pentyl-2-piperidinone, 9CI

[200940-76-7]



$C_{13}H_{23}NO_2$ 225.33

(R)-form [175669-30-4]

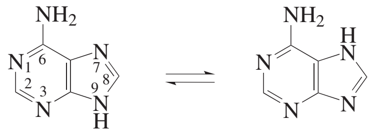
Alkaloid from the European ladybird beetles *Adalia bipunctata* and *Adalia decempunctata*. Oil. $[\alpha]_{579}^{20}$ -26 (c, 0.13 in CH_2Cl_2) (natural). $[\alpha]_D^{20}$ -28.3 (c, 1.6 in CH_2Cl_2) (synthetic).

Lognay, G. *et al., J. Nat. Prod.*, 1996, **59**, 510-511 (*isol, ir, pmr, cmr, ms, struct*)

Broeders, F. *et al., Bull. Soc. Chim. Belg.*, 1997, **106**, 377-382 (*synth*)
Yamazaki, N. *et al., Tet. Lett.*, 1999, **40**, 739-742 (*synth, abs config*)
Honda, T. *et al., Org. Lett.*, 2000, **2**, 3925-3927 (*synth*)
Laurent, P. *et al., Tetrahedron*, 2001, **57**, 3403-3412 (*biosynth*)

Adenine, JAN, USAN A-137

*1*H-*Purin-6-amine, 9CI. 6-Aminopurine. Vitamin B$_4$. Angustmycin B*
[73-24-5]



9*H-form* 7*H-form*

$C_5H_5N_5$ 135.128

9*H*-form is favoured in free base. CAS refers mainly to 1*H* struct. which is not in reality a favoured tautomer. Widespread throughout animal and plant tissue, purine components of DNA, RNA, and coenzymes and biosynthetic intermediates. Antiviral agent, granulocyte antagonist.Vitamin. Pharmaceutical aid used to extend storage life of whole blood. Needles + $3H_2O$ (H_2O). Mp 360-365° (anhyd.) dec. pK_{a1} 4.12; pK_{a2} 9.83 (25°).

▶ Exp. reprod. and teratogenic effects. LD$_{50}$ (rat, orl) 745 mg/kg. AU6125000

Hydrochloride: [2922-28-3]
Cryst. + $0.5H_2O$. Mp 285°.

6N-*Me: 6-(Methylamino)purine*
[443-72-1]
$C_6H_7N_5$ 149.155
Minor constit. of bacterial and viral DNA. Mp 312-314° dec. pK_{a1} 4.18; pK_{a2} 9.99 (H_2O).

6N-*Benzyl:* N-*Benzyladenine, 8CI. 6-Benzylaminopurine.* ***Cytokinin B****. BAP*
[1214-39-7]
$C_{12}H_{11}N_5$ 225.252
Widespread in plants. Plant growth regulator. Cryst. (C_6H_6). Mp 229°.

▶ AU6252200

6N-*(3-Hydroxybenzyl):* 6N-*(3-Hydroxybenzyl)adenine.* **meta-*Topolin***
$C_{12}H_{11}N_5O$ 241.252
Isol. from *Populus* x *canadensis* cv. *robusta*. Cytokinin. No phys. props. reported.

1*H-form*

1-(3-Methyl-2-butenyl): 1-(3-Methyl-2-butenyl)adenine. ***1-Prenyladenine***
$C_{10}H_{13}N_5$ 203.246
Constit. of the leaves of *Bridelia balansae*. Prisms. Mp >300°. λ_{max} 209 (log ϵ 4.13); 274 (log ϵ 4.04) (MeOH).

3*H-form*

3-(3-Methyl-2-butenyl): see Triacanthine, T-451

9*H-form*

6N-*Me, 9-*O*-β-*D*-glucopyranosyl:*
[253179-56-5]
$C_{12}H_{17}N_5O_5$ 311.297
Constit. of *Maerua crassifolia*.

6N-*(3-Hydroxybenzyl), 9-β-*D*-glucopyranosyl:* **meta-*Topolin 9-glucoside***
$C_{18}H_{21}N_5O_6$ 403.394
Isol. from *Populus* x *canadensis* cv. *robusta*. Cytokinin. No phys. props. reported.

N^9-*(3-Methyl-2-butenyl): 9-(3-Methyl-2-butenyl)adenine. 9-Prenyladenine*
$C_{10}H_{13}N_5$ 203.246
Constit. of the leaves of *Bridelia balansae*. Prisms. Mp 188-189°. λ_{max} 212 (log ϵ 4.1); 274 (log ϵ 2.8) (MeOH).

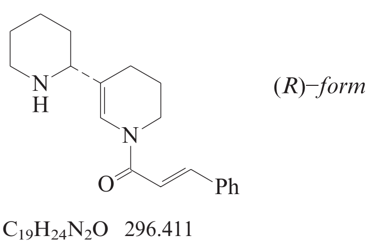
N^9-*[1-(3,4-Dihydroxyphenyl)ethyl]: 6-Amino-9-[1-(3,4-dihydroxyphenyl)ethyl]purine. 9-[1-(3,4-Dihydroxyphenyl)ethyl]adenine*
$C_{13}H_{13}N_5O_2$ 271.278
Isol. from *Artemisia capillaris*. Amorph. powder.

[6055-72-7 , 2312-73-4]

Skinner, C.G. *et al., J.A.C.S.*, 1955, **77**, 6692-6693 (*Cytokinin B*)
Dunn, D.B. *et al., Biochem. J.*, 1958, **68**, 627-636 (*isol, 6-Methylaminopurine*)
Kistenmacher, T.J. *et al., Acta Cryst. B*, 1974, **30**, 166-168; 1528-1533; 1977, **33**, 253-256 (*cryst struct, 9-Me*)
Lawley, P.D. *et al., Biochem. J.*, 1975, **145**, 73-84 (*ms, derivs*)
Chenon, M.T. *et al., J.A.C.S.*, 1975, **97**, 4636-4642 (*cmr, tautom*)
Kos, N.J. *et al., J.O.C.*, 1979, **44**, 3140-3143 (*synth, nmr*)
Lin, J. *et al., J.A.C.S.*, 1980, **102**, 4627-4631 (*pe, tautom*)
Mathlouth, M. *et al., Carbohydr. Res.*, 1984, **131**, 1-15 (*ir, Raman*)
Remaud, G. *et al., Tetrahedron*, 1986, **42**, 5073-5080 (*N-15 nmr, derivs*)
Strnad, M. *et al., Phytochemistry*, 1997, **45**, 213-218 (*meta-Topolin*)
Ramadan, M.A. *et al., CA*, 2000, **132**, 61604r (*6-N-Me-9-glucosyl*)
Tsai, Y.H. *et al., Helv. Chim. Acta*, 2003, **86**, 2452-2457 (*Bridelia prenyladenines*)
Ma, H.-Y. *et al., Molecules*, 2008, **13**, 267-271 (*9-N-Dihydroxyphenylethyl*)

Adenocarpine A-138

1,2,3,4-Tetrahydro-1-(1-oxo-3-phenyl-2-propenyl)-5-(2-piperidinyl)pyridine, 9CI. 1′-Cinnamoyl-1,1′,2,3,4,4′,5,5′,6,6′-decahydro-2,3′-bipyridine. N*-Cinnamoyl-Δ^2-tetrahydroanabasine. Orensine. Teidine*
[6793-63-1]



$C_{19}H_{24}N_2O$ 296.411

(*R*)-*form* [28052-98-4]
Alkaloid from *Adenocarpus commutatus* and *Adenocarpus grandiflorus* (Fabaceae). $[\alpha]^{18}_D$ -30.9 (c, 2 in EtOH).

Hydrochloride: Mp 64-65°.

Picrate: Mp 206° dec.

(*S*)-*form* [28976-53-6]
Alkaloid from *Adenocarpus complicatus, Adenocarpus foliosus* and *Adenocarpus viscosus* (Fabaceae). Resin. $[\alpha]^{18}_D$ +29.3 (c, 2 in EtOH).

Hydrochloride: Mp 65° (hydrate) Mp 133-147° dec. (anhyd.).

Picrate: Mp 213°.

(±)-*form* [494-06-4]
Alkaloid of *Adenocarpus commutatus* and *Adenocarpus grandiflorus* (Fabaceae). Resin or pale-yellow oil.

Hydrochloride: Mp 208-210° Mp 82-83° (dihydrate).

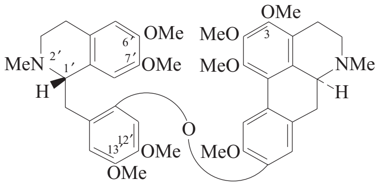
Picrate: Mp 210-211° dec.

(Z)-Cinnamoyl isomer: ***Isoorensine***
[28168-92-5]
$C_{19}H_{24}N_2O$ 296.411
Alkaloid from *Adenocarpus complicatus* leaves (Fabaceae).

Ribas, I. *et al., An. R. Soc. Esp. Fis. Quim., Ser. B*, 1950, **46**, 489; 1951, **47**, 533; 1953, **49**, 707; 1955, **51**, 55; 1958, **54**, 157; 215 (*isol, struct, resoln, Isoorensine*)
González, A.G. *et al., An. R. Soc. Esp. Fis. Quim., Ser. B*, 1951, **47**, 67; 1953, **49**, 783
Ribas, I. *et al., Ann. Pharm. Fr.*, 1952, **19**, 54 (*isol*)
Schöpf, C. *et al., Annalen*, 1964, **674**, 87 (*synth*)
Schöpf, C. *et al., Naturwissenschaften*, 1966, **53**, 274 (*Isoorensine*)
Fitch, W.L. *et al., J.A.C.S.*, 1974, **96**, 4917 (*ms*)
Nehme, M. *et al., An. Quim.*, 1977, **73**, 307 (*isol*)

Adiantifoline A-139

[20823-96-5]



$C_{42}H_{50}N_2O_9$ 726.865
Alkaloid from the roots and tops of *Thalictrum minus* var. *adiantifolium*, the underground parts of *Thalictrum minus* var. *microphyllum* and the roots of *Thalictrum minus* race B (Ranunculaceae). Pale-yellow needles (EtOH). Mp 143.5-144°. $[\alpha]^{28}_D$ +90 (c, 0.11 in MeOH).

*2′-*N*-De-Me:* ***2′-Noradiantifoline***
[83348-50-9]
$C_{41}H_{48}N_2O_9$ 712.838
Alkaloid from the roots and rhizomes of *Thalictrum minus* (Ranunculaceae). Amorph. $[\alpha]^{25}_D$ +39 (c, 0.082 in MeOH).

O^3*-De-Me:* ***Thalilutine***
[66408-21-7]
$C_{41}H_{48}N_2O_9$ 712.838
Minor alkaloid from *Thalictrum revolutum* roots (Ranunculaceae). Amorph. $[\alpha]^{20}_D$ +92 (c, 0.175 in MeOH).

O$^{6′}$*-De-Me:* **O$^{6′}$*-Demethyladiantifoline***

$C_{41}H_{48}N_2O_9$ 712.838
Alkaloid from the roots of *Thalictrum minus* (Ranunculaceae). Mp 125-126°. $[\alpha]_D^{22}$ +18 (c, 0.4 in $CHCl_3$).

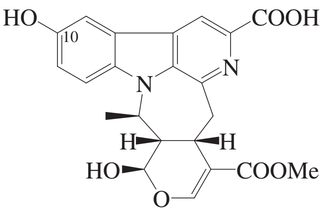
O$^{7'}$*-De-Me:* ***Thaliadanine***
[31199-54-9]
$C_{41}H_{48}N_2O_9$ 712.838
Alkaloid from *Thalictrum minus* roots and from *Thalictrum minus* var. *microphyllum* (Ranunculaceae). Shows antibacterial activity against *Mycobacterium smegmatis*. Amorph. $[\alpha]_D^{26}$ +81 (c, 0.41 in MeOH). λ_{max} 281 ; 302 ; 312 (MeOH) (Berdy).

O$^{7'}$,O$^{13'}$*-Di-de-Me:* ***Bursanine***
[82958-13-2]
$C_{40}H_{46}N_2O_9$ 698.811
Alkaloid from the roots and rhizomes of *Thalictrum minus* var. *microphyllum* (Ranunculaceae). $[\alpha]_D^{25}$ +117 (c, 0.17 in MeOH).

Doskotch, R.W. *et al., Tet. Lett.*, 1968, 4999; *J. Nat. Prod.*, 1969, **32**, 29 (*isol, uv, cd, pmr, ms, struct*)
Mollov, N.M. *et al., CA*, 1971, **74**, 61584t (*isol, ir, pmr, O-Demethyladiantifoline*)
Doskotch, R.W. *et al., J.O.C.*, 1971, **36**, 2409 (*synth*)
Geiselman, C.W. *et al., J. Nat. Prod.*, 1972, **35**, 296 (*isol*)
Shamma, M. *et al., Tet. Lett.*, 1973, 1859 (*pmr*)
Wu, W.-N. *et al., Tetrahedron*, 1977, **33**, 2919 (*uv, cd, pmr, ir, ms, struct, Thalilutine*)
Liao, W.T. *et al., J. Nat. Prod.*, 1978, **41**, 271 (*isol, uv, cd, ir, pmr, ms, struct, O-Demethyladiantifoline, Th*)
Guinaudeau, H. *et al., J. Nat. Prod.*, 1982, **45**, 505 (*uv, cd, pmr, ms struct, Noradiantifoline*)
Guinaudeau, H. *et al., Tet. Lett.*, 1982, **23**, 2523 (*uv, pmr, ms, cd, struct, Bursanine*)

Adifoline A-140

[20072-28-0]



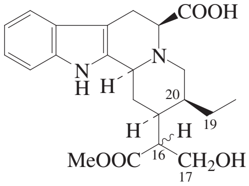
$C_{22}H_{20}N_2O_7$ 424.409
Recent work has queried the struct. It is suggested, but not proved, that the prev. isolated Adifoline is identical with Neoadifoline, N-98. Alkaloid from the heartwood of *Adina cordifolia* (Rubiaceae). Yellow needles. Mp 300°.

10-Deoxy: ***Deoxyadifoline***
[21451-49-0]
$C_{22}H_{20}N_2O_6$ 408.41
Alkaloid from *Adina cordifolia* (Rubiaceae). Mp 253-255° (as Ac, Me ester). $[\alpha]_D^{20}$ +560 (c, 0.105 in $CHCl_3$) (Ac, Me ester).

Cross, A.D. *et al., J.C.S.*, 1961, 2714 (*isol, uv, ir*)
Brown, R.T. *et al., Chem. Comm.*, 1968, 350 (*uv, ir, pmr, ms, struct*)
Merlini, L. *et al., Gazz. Chim. Ital.*, 1968, **98**, 974 (*Deoxyadifoline*)
Balázs, B. *et al., Magn. Reson. Chem.*, 1999, **37**, 751-753

Adirubine A-141

[38474-14-5]



Absolute Configuration

$C_{22}H_{28}N_2O_5$ 400.474
Alkaloid from *Adina rubescens* (Rubiaceae).

Me ester: $[\alpha]_D^{25}$ -34 ($CHCl_3$).

O*-Ac:* Mp 151-154°. $[\alpha]_D^{25}$ -19 ($CHCl_3$).

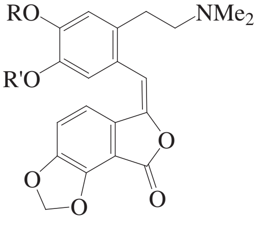
*19*E*,20-Didehydro,* O*-Ac:* ***19,20-Dehydroadirubine acetate***
[77485-21-3]
$C_{24}H_{28}N_2O_6$ 440.495
Trace alkaloid from the leaves of *Rauwolfia oreogiton* (Apocynaceae). Off-white amorph. powder. λ_{max} 227 (log ϵ 4.4); 285 (log ϵ 3.8); 291 (log ϵ 3.82) (MeOH).

17-Deoxy, 16,17-didehydro: ***Anhydroadirubine***
[58514-04-8]
$C_{22}H_{26}N_2O_4$ 382.458
Alkaloid from *Adina rubescens* (Rubiaceae). Amorph. powder (as Me ester). $[\alpha]_D^{25}$ -28 ($CHCl_3$) (Me ester). λ_{max} 225 ; 273 ; 282 ; 289 (MeOH) (Me ester).

Brown, R.T. *et al., Chem. Comm.*, 1972, 1007-1008; 1976, 530-531 (*ir, pmr, ms, struct, config*)
Brown, R.T. *et al., Phytochemistry*, 1975, **14**, 2527-2529 (*Anhydroadirubine*)
Van Tamelen, E.E. *et al., Bioorg. Chem.*, 1976, **5**, 283-308 (*ester, synth*)
Akinloye, B.A. *et al., Phytochemistry*, 1980, **19**, 2741-2745 (*19,20-Dehydroadirubine acetate*)

Adlumiceine enol lactone A-142

*6-[[2-[2-(Dimethylamino)ethyl]-4,5-dimethoxyphenyl]methylene]furo[3,4-*e*]-1,3-benzodioxol-8(6*H*)-one, 9CI*
[75832-77-8]



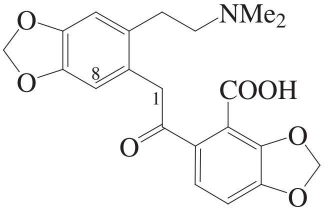
R = R' = Me

$C_{22}H_{23}NO_6$ 397.427
Alkaloid from *Fumaria schrammii.*

Popova, M. *et al., Planta Med.*, 1980, **40**, 156

Adlumidiceine A-143

5-[[6-[2-(Dimethylamino)ethyl]-1,3-benzodioxol-5-yl]acetyl]-1,3-benzodioxole-4-carboxylic acid, 9CI
[51059-65-5]



$C_{21}H_{21}NO_7$ 399.399
Alkaloid from *Corydalis sempervirens* (*Corydalis glauca*), *Corydalis cava* (*Corydalis tuberosa*), *Corydalis lutea*, *Fumaria schrammii* and *Papaver rhoeas* (corn poppy) (Papaveraceae, Papaveraceae). Cryst. (MeOH). Mp 244-246°.

1-Hydroxy: ***Narceimicine***
[116368-95-7]
$C_{21}H_{21}NO_8$ 415.399
Alkaloid from the seeds of *Fumaria indica* (Papaveraceae). Pale-yellow granules (MeOH aq.). Mp 242-246° dec. Shown in the paper as the enediol tautomer.

1-Hydroxy, Me ester: ***Paprafumine***
[169626-17-9]
$C_{22}H_{23}NO_8$ 429.426
Alkaloid from aerial parts of *Fumaria indica* (Papaveraceae). Amorph. solid. Shown in the paper as the enediol tautomer.

1-Oxo: ***Narceimine****. Bicucullinine. Alkaloid F45*
[59443-00-4]
$C_{21}H_{19}NO_8$ 413.383
Alkaloid from *Fumaria indica* and *Corydalis ochroleuca* (Papaveraceae). Mp 268° (259-260°).

1-Oxo, Me ester: Mp 188°.

1-Oxo, N*-Me:* **N*-Methylnarceimine***. N*-Methylnarceimicine (incorr.)*
[777007-71-3]
$C_{22}H_{22}NO_8^{\oplus}$ 428.418
Quaternary alkaloid from *Corydalis saxicola*. Yellow cryst. (MeOH). Mp 194-196°. Counterion not specified. λ_{max} 207 (log ϵ 4.48); 331 (log ϵ 4.02) (MeOH).

Preininger, V. *et al., Phytochemistry*, 1973, **12**, 2513 (*ir, uv, pmr, ms, struct*)
Preininger, V. *et al., Coll. Czech. Chem. Comm.*, 1975, **40**, 699 (*ir, uv, pmr, ms, struct*)
Rodrigo, R.G.A. *et al., Can. J. Chem.*, 1976, **54**, 471 (*isol, ir, pmr, cmr, ms, struct, Narceimine*)
Seth, K.K. *et al., Chem. Ind. (London)*, 1979, 744 (*ir, uv, pmr, ms, struct, Narceimine*)
Popova, M.E. *et al., Planta Med.*, 1982, **45**, 120 (*isol*)
Tripathi, Y.C. *et al., Phytochemistry*, 1988, **27**, 1918 (*Narceimicine, isol, ir, uv, pmr, ms, struct*)
Atta-ur-Rahman, *et al., Phytochemistry*, 1995, **40**, 593 (*Parafumine*)
Wu, Y.-R. *et al., Planta Med.*, 2007, **73**, 787-791 (*N-Methylnarceimine*)

Adlumidiceine enol lactone A-144

*6-[[6-[2-(Dimethylamino)ethyl]-1,3-benzodioxol-5-yl]methylene]furo[3,4-*e*]-1,3-benzodioxol-8(6*H*)-one, 9CI*

As Adlumiceine enol lactone, A-142 with R,R′ = –CH₂-

$C_{21}H_{19}NO_6$ 381.384

(E)-form [51059-67-7]

Alkaloid from *Fumaria schrammii, Corydalis sempervirens, Corydalis ochotensis* and *Corydalis lutea* (Papaveraceae). Cryst. (Et_2O). Mp 200-203°.

(Z)-form

Aobamidine

[59614-38-9]

Alkaloid from *Corydalis ochotensis* and *Corydalis lutea* (Papaveraceae). Yellowish powder (Et_2O). Mp 195-197°.

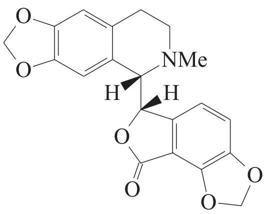
Preininger, V. *et al., Phytochemistry*, 1973, **12**, 2513 (*uv, ir, pmr, struct*)

Kametani, T. *et al., J.C.S. Perkin 1*, 1977, 390 (*isol, uv, ir, pmr, ms, struct*)

Preininger, V. *et al., Planta Med.*, 1978, **33**, 396 (*isol*)

Adlumidine A-145

*6-(5,6,7,8-Tetrahydro-6-methyl-1,3-dioxolo[4,5-*g*]isoquinolin-5-yl)furo[3,4-*e*]-1,3-benzodioxol-8(6*H*)-one, 9CI*



(+)–*form*

$C_{20}H_{17}NO_6$ 367.357

Diastereoisomer of Bicuculline, B-119.

(+)-form [550-49-2]

Alkaloid from *Corydalis decumbens, Corydalis gigantea, Corydalis incisa, Corydalis ochotensis, Corydalis ochroleuca, Corydalis remota, Corydalis sibirica, Corydalis thalictrifolia, Fumaria indica, Fumaria parviflora* and *Adlumia fungosa* (*Adlumia cirrhosa*)(Papaveraceae, Papaveraceae). Cryst. (Me_2CO). Mp 239-240° (237°). $[\alpha]_D^{20}$ +116.2 (c, 2 in $CHCl_3$).

▶AV3085000

(-)-form

Capnoidine

[485-50-7]

Alkaloid from *Corydalis cava, Corydalis crystallina, Corydalis gigantea, Corydalis gortschakovii, Corydalis marshalliana, Corydalis pseudo-adunca, Corydalis sempervirens* and *Fumaria vaillantii* (Papaveraceae). Cryst. ($CHCl_3$/MeOH). Mp 239° (235°). $[\alpha]_D^{22}$ -113.2 (c, 0.8 in $CHCl_3$) (-100).

▶EX8585000

(±)-form [64397-08-6]

Alkaloid from *Corydalis rosea*. Cryst. ($CHCl_3$/MeOH, MeOH or C_6H_6/Me_2CO). Mp 205° (184-186°, 198-199°).

Manske, R.H.F. *et al., J.A.C.S.*, 1950, **32**, 3207 (*isol, struct*)

Bláha, K. *et al., Coll. Czech. Chem. Comm.*, 1964, **29**, 2328 (*config*)

Snatzke, G. *et al., Tetrahedron*, 1969, **25**, 5059 (*ord, cd*)

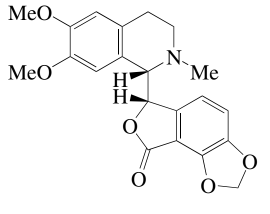
Margvelashvili, N.N. *et al., Khim. Prir. Soedin.*, 1972, **8**, 127; 1978, **14**, 592; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 131; 1978, **14**, 509 (*isol, ir, uv*)

Lu, S.-T. *et al., J.C.S. Perkin 1*, 1976, 63 (*isol*)

Blaskó, G. *et al., J. Nat. Prod.*, 1982, **45**, 121 (*occur*)

Ribár, B. *et al., Acta Cryst. C*, 1991, **47**, 2191 (*cryst struct*)

Adlumine A-146



(+)-*form*

$C_{21}H_{21}NO_6$ 383.4

Diastereoisomer of Corlumine, C-653.

(+)-form [524-46-9]

Alkaloid from *Adlumia fungosa* (*Adlumia cirrhosa*) and *Fumaria rostellata* (Papaveraceae, Papaveraceae). Mp 180°. $[\alpha]_D$ +42 ($CHCl_3$).

(-)-form [21414-43-7]

Alkaloid from *Corydalis scouleri, Corydalis ophiocarpa, Corydalis rosea, Corydalis gortschakovii, Corydalis gigantea, Corydalis sempervirens, Fumaria kralikii, Fumaria parviflora* and *Fumaria vaillantii* (Papaveraceae). Cryst. ($CHCl_3$ or $CHCl_3$/MeOH). Mp 178-180°. $[\alpha]_D^{20}$ -42 (c, 0.38 in $CHCl_3$). $[\alpha]_D^{20}$ -51.

N-*Me:* **N-*Methyladlumine***

[80550-26-1]

$C_{22}H_{24}NO_6^{\oplus}$ 398.435

Quaternary alkaloid from *Fumaria vaillantii*. Cryst. (MeOH) (as iodide). Mp 198-199° (iodide). $[\alpha]_D$ -45 (c, 0.5 in MeOH) (iodide).

O^6-*De-Me:* ***Corledine***

$C_{20}H_{19}NO_6$ 369.373

Alkaloid from *Corydalis ledebouriana* (Papaveraceae). Cryst. (MeOH). Mp 210-212°. $[\alpha]_D$ -100 (c, 0.2 in MeOH). Methylation gives Adlumine.

O^7-*De-Me:* ***Severtzine***. l-*Adlumine. Severcine*

[59272-73-0]

$C_{20}H_{19}NO_6$ 369.373

Alkaloid from *Corydalis severtzovii* (Papaveraceae). Cryst. (MeOH). Mp 94-95° (foams). $[\alpha]_D$ -52 (c, 0.91 in $CHCl_3$).

(±)-form [38184-69-9]

Alkaloid from *Corydalis rosea* (Papaveraceae). Mp 191° (175°, 184-186°).

Safe, S. *et al., Can. J. Chem.*, 1964, **42**, 160 (*pmr, config*)

Snatzke, G. *et al., Tetrahedron*, 1969, **25**, 5059 (*ord*)

Margvelashvili, N.N. *et al., Khim. Prir. Soedin.*, 1972, **8**, 127; 1976, **12**, 832; 1978, **14**, 592; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 131; 1976, **12**, 509; 1978, **14**, 754 (*isol, ir, uv*)

Shamma, M. *et al., Tet. Lett.*, 1974, 2339 (*synth, pmr*)

Preininger, V. *et al., Coll. Czech. Chem. Comm.*, 1975, **40**, 699 (*isol*)

Israilov, I.A. *et al., Khim. Prir. Soedin.*, 1975, **11**, 811; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 826 (*Severtzine*)

Hughes, D.W. *et al., Can. J. Chem.*, 1976, **54**, 2252 (*cmr*)

Nalliah, B.C. *et al., Can. J. Chem.*, 1977, **55**, 922; 1979, **57**, 1546 (*synth*)

Moiseeva, G.P. *et al., Khim. Prir. Soedin.*, 1978, **14**, 103; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 82 (*cd*)

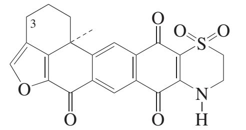
Alimova, M. *et al., Khim. Prir. Soedin.*, 1981, **17**, 602-604; *Chem. Nat. Compd. (Engl. Transl.)*, 1981, **17**, 437-438 (*N-Methyladlumine*)

Blaskó, G. *et al., J. Nat. Prod.*, 1982, **45**, 105 (*occur*)

Seger, C. *et al., Magn. Reson. Chem.*, 2004, **42**, 882-886 (*pmr, cmr*)

Adociaquinone B A-147

[113831-00-8]



Absolute Configuration

$C_{22}H_{17}NO_6S$ 423.445

Isol. from the sponges *Adocia* and *Xestospongia* spp. Mildly cytotoxic. Topoisomerase inhibitor. Yellow solid. $[\alpha]_D$ +22. Slowly dec. >300°. λ_{max} 288 (ϵ 36000); 340 (ϵ 12000) (EtOH) (Derep). λ_{max} 294 (ϵ 14400) (MeOH) (Berdy).

3-Oxo: ***3-Oxoadociaquinone B***. *3-Ketoadociaquinone B*

[848242-73-9]

$C_{22}H_{15}NO_7S$ 437.429

Isol. from a *Xestospongia* sp. Yellowish powder. $[\alpha]_D^{23}$ +13 (c, 0.12 in MeOH). λ_{max} 273 (log ϵ 3.6) (MeOH).

Schmitz, F.J. *et al., J.O.C.*, 1988, **53**, 3922-3925 (*isol, pmr, cmr*)

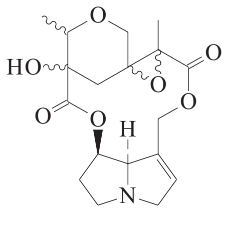
Concepcion, G.P. *et al., J. Med. Chem.*, 1995, **38**, 4503-4507 (*isol*)

Harada, N. *et al., Tetrahedron: Asymmetry*, 1995, **6**, 375-376 (*synth, abs config*)

Cao, S. *et al., Bioorg. Med. Chem.*, 2005, **13**, 999-1003 (*3-Oxoadociaquinone B*)

Adonifoline A-148

[115712-88-4]



$C_{18}H_{23}NO_7$ 365.382

Revised struct. (1992). Two previous

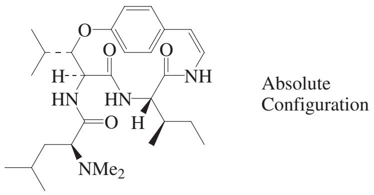
isolates shown to be identical with the alkaloid now named Adonifoline. Alkaloid from *Senecio adonidifolius* and *Senecio dolichodoryius* (Asteraceae). Cryst. (Me_2CO). Mp 200°. $[\alpha]_D$ +84.74 (c, 0.78 in MeOH).

Witte, L. *et al., Phytochemistry*, 1992, **31**, 1027-1028 (*isol, pmr, cmr, ms*)

Adouetine X A-149

Ceanothamine B

[19542-37-1]



$C_{28}H_{44}N_4O_4$ 500.68

Alkaloid from *Waltheria americana*, the root bark of *Ceanothus americanus* (New Jersey tea) and *Zizyphus jujuba* var. *inermis*, and the leaves of *Alphitonia macrocarpa* (Sterculiaceae, Rhamnaceae). Needles (MeOH or CH_2Cl_2/EtOAc). Mp 279-280.5°. $[\alpha]_D^{25}$ -370 (c, 0.205 in $CHCl_3$).

N-*De-Me:* ***Discarine F***. N-*Demethyladouetine X*

[96562-84-4]

$C_{27}H_{42}N_4O_4$ 486.653

Alkaloid from the bark of *Discaria febrifuga* (Rhamnaceae). Mp 264°. $[\alpha]_D^{20}$ -191 ($CHCl_3$).

Païs, M. *et al., Ann. Pharm. Fr.*, 1963, **21**, 139-146; *CA*, **59**, 5215c (*isol, ir, pmr*)

Warnhoff, E.W. *et al., Can. J. Chem.*, 1965, **43**, 2594-2602 (*isol, uv, ms, pmr*)

Païs, M. *et al., Bull. Soc. Chim. Fr.*, 1968, 1145-1148 (*uv, ir, pmr, ms, struct*)

Servis, R.E. *et al., J.A.C.S.*, 1969, **91**, 5619-5624 (*isol, ms*)

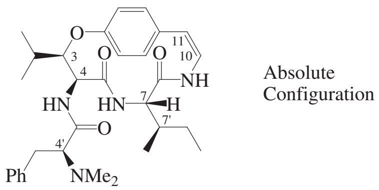
Branch, G.B. *et al., Aust. J. Chem.*, 1972, **25**, 2209-2216 (*isol*)

Otsuka, H. *et al., Phytochemistry*, 1974, **13**, 2016 (*isol, ir, pmr, ms*)

Morel, A. *et al., Z. Naturforsch., B*, 1984, **39**, 1825 (*Discarine F*)

Adouetine Y′ A-150

[19542-39-3]



$C_{31}H_{42}N_4O_4$ 534.697

Alkaloid from *Waltheria americana*, *Waltheria douradhina*, *Myrianthus arboreus*, *Melochia corchorifolia*, *Discaria longispina*, *Discaria febrifuga*, *Discaria americana* and *Ceanothus sanguineus*. Cryst. ($CHCl_3/Et_2O$). Mp 295-297°. $[\alpha]_D^{20}$ -390 (c, 1 in $CHCl_3$).

N-*De-Me:* **N-*Demethyladouetine Y′***

[73045-49-5]

$C_{30}H_{40}N_4O_4$ 520.67

Alkaloid from the root bark of *Ceanothus sanguineus* (Rhamnaceae). Mp 229°. Opt. rotn. not recorded.

10,11-Dihydro, 11-hydroxy: ***Discarine G***

[94901-64-1]

$C_{31}H_{44}N_4O_5$ 552.712

Alkaloid from the root bark of *Discaria febrifuga* (Rhamnaceae). Mp 257°. $[\alpha]_D^{20}$ -366 (c, 0.1 in MeOH). Stereochem. not determined.

Stereoisomer (1): ***Lotusanine A***

[164455-28-1]

$C_{31}H_{42}N_4O_4$ 534.697

Alkaloid from *Zizyphus lotus*. Amorph. solid. Has (3*R*,4*R*)-config. with the other centres unassigned. Stated to be racemic. λ_{max} 208 (log ε 4.2) (MeOH).

Stereoisomer (2): ***Myrianthine B***. *Alkaloid AM 1*

[24532-77-2]

$C_{31}H_{42}N_4O_4$ 534.697

Alkaloid from *Myrianthus arboreus* and leaves of *Antidesma montana*. Needles (MeOH). Mp 302° dec. (292°). $[\alpha]_D$ -360 (c, 0.14 in $CHCl_3$) (-294). Has (4*S*,7*S*)-config. with the other centres undetermined.

Marchand, J. *et al., Ann. Pharm. Fr.*, 1968, **26**, 771-778; *CA*, **71**, 42203q (*Myrianthine B*)

Païs, M. *et al., Bull. Soc. Chim. Fr.*, 1968, 1145-1148 (*uv, ir, pmr, ms, struct*)

Tschesche, R. *et al., Tet. Lett.*, 1968, 3817-3818 (*isol, ms*)

Merkuza, V.M. *et al., Phytochemistry*, 1974, **13**, 1279-1282 (*ir, ms*)

Lagarias, J.C. *et al., J. Nat. Prod.*, 1979, **42**, 663-668 (*N-Demethyladouetine Y′*)

Herzog, R. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1984, **365**, 1351-1354 (*Discarine G*)

Arbain, D. *et al., Phytochemistry*, 1993, **33**, 1263-1266 (*AM-1*)

Abu-Zarga, M. *et al., J. Nat. Prod.*, 1995, **58**, 504-511 (*Lotusanine A*)

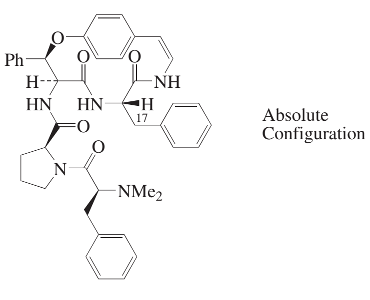
Da Silva, U.F. *et al., Phytochem. Anal.*, 1996, **7**, 20-23 (*config*)

Tan, N.H. *et al., Chem. Rev.*, 2006, **106**, 840-895 (*bibl*)

Adouetine Z A-151

N,N-*Dimethylphenylalanyl*-N-*[5,8-dioxo-3-phenyl-7-(phenylmethyl)-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]prolinamide, 9CI*. N-*Methylferetine. Adouetine*

[19542-40-6]



$C_{42}H_{45}N_5O_5$ 699.848

Alkaloid from *Waltheria americana*, and from the leaves of *Feretia apodanthera* and *Melochia pyramidata* (Sterculiaceae, Rubiaceae). Cryst. (cyclohexane). Mp 135-140° Mp 140-145°. $[\alpha]_D$ -184 (c, 1 in $CHCl_3$).

▶ TW3577000

N-*De-Me:* ***Feretine***. N-*Demethyladouetine Z*

[56031-09-5]

$C_{41}H_{43}N_5O_5$ 685.821

Alkaloid from the leaves of *Feretia apodanthera* (Rubiaceae). Cryst. (cyclohexane). Mp 123°. $[\alpha]_D$ -139 (c, 1 in $CHCl_3$).

10,11-Dihydro:

Cryst. (Me_2CO/hexane). Mp 221°. $[\alpha]_D$ -87 ($CHCl_3$).

17-Hydroxy: ***Oxyphylline A***

[959855-77-7]

$C_{42}H_{45}N_5O_6$ 715.847

Alkaloid from the stem bark of *Zizyphus oxyphylla*. Cryst. Mp 204-206°. λ_{max} 233 (MeOH).

Païs, M. *et al., Ann. Pharm. Fr.*, 1963, **21**, 139-146; *CA*, **59**, 5215c (*isol, ir, pmr*)

Païs, M. *et al., Bull. Soc. Chim. Fr.*, 1968, 1145-1148 (*uv, ir, pmr, ms, struct*)

Bailleul, F. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1974, **279**, 949-951 (*Feretine*)

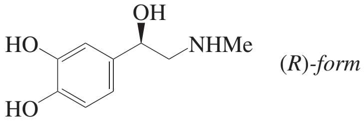
Medina, E. *et al., Annalen*, 1981, 538-545 (*isol, ir, cmr, ms*)

Inayat-ur-Rahman, *et al., Nat. Prod. Res.*, 2007, **21**, 243-253 (*Oxyphylline A*)

Adrenaline, BAN A-152

4-[1-Hydroxy-2-(methylamino)ethyl]-1,2-benzenediol, 9CI. 3,4-Dihydroxy-α-[(methylamino)methyl]benzyl alcohol, 8CI. 1-(3,4-Dihydroxyphenyl)-2-methylaminoethanol. ***Epinephrine, INN, USAN***. *Bronkaid. Epifrin. Glaucon. Bosmin. Suprarenin. NSC 62786*

[6912-68-1]



$C_9H_{13}NO_3$ 183.207

Used in photometric detn. of Ti. Active constit. of the adrenal gland. α,β-Adrenoceptor agonist, vasoconstrictor, inotropic agent. Mydriatic. Used in management of anaphylaxis, and in cardiopulmonary resuscitation. Orally inactive. Used in combination with fluorouracil in the treatment of genital warts (AccuSite). Log P -0.68 (calc). First hormone to be isol. (in 1856) and synthesised (1904).

▶ May cause contact dermatitis.

(R)-form

L-form (obsol.)

[51-43-4]

Powder. Sol. alkalis, acids; spar. sol. H_2O, EtOH; insol. Et_2O. Mp 216° dec. $[\alpha]_D^{20}$ -53 (c, 4 in 1*M* HCl). Pharmacol. more active isomer.

▶ LD_{50} (rat, skn) 62 mg/kg. LD_{50} (rat, ivn)

0.15 mg/kg. DO2625000

Hydrochloride: [55-31-2]
Mp 157°.

▶ DO3150000

Tartrate: ***Epinephrine bitartrate, USAN****. Epitrate*
[51-42-3]
[24351-82-4] Ophthalmic adrenergic agent. Cryst. Mp 147-154°.

▶ DO3500000

Cyclic borate: ***Epinephryl borate, USAN****. Epinal*†*. Epinephrine borate*
[5579-16-8] Ophthalmic adrenergic agent.

N-*Me: 4-[2-(Dimethylamino)-1-hydroxyethyl]-1,2-benzenediol, 9CI.* **N-*Methyladrenaline***
[554-99-4]
$C_{10}H_{15}NO_3$ 197.233
Alkaloid from tubers of *Aconitum nasutum* (Ranunculaceae).

▶ DO5425000

N-*De-Me:* see Norepinephrine, N-298

O^3,O^4,N-*Tri-Me:* see Macromerine, M-18

(*S*)-*form*

D-form (obsol.)
[150-05-0]
Light brown cryst. Mp 211-212°. About 12 times less hormonally active than the (*R*)-enantiomer.

▶ DO2800000

(±)-*form*

Racepinefrine, INN*. Racepinephrine, USAN. Vaponephrin*
[329-65-7]
Microscopic cryst. Sl. sol. H_2O. Mp 230° dec.

▶ DO2975000

Hydrochloride: Racepinephrine hydrochloride, USAN
[329-63-5]
Cryst. (EtOH). Mp 157°.

▶ DO3330000

Di-Ac:
$C_{13}H_{17}NO_5$ 267.281
Mp 168°.

Di-Ac; hydrochloride: Mp 155-156°.

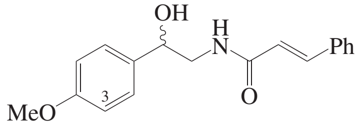
(ξ)-*form*

Isol. from callus tissue of *Portulaca grandiflora*.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1296A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 625B (*nmr*)
Vulpian, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1856, **43**, 663-665 (*isol*)
Stolz, F. *et al., Ber.*, 1904, **37**, 4149-4154 (*synth*)
Ciocca, B. *et al., Boll. Chim. Farm.*, 1934, **73**, 241-245; *CA*, **28**, 4398 (*synth*)
Pratesi, P. *et al., J.C.S.*, 1959, 4062-4065 (*abs config*)
Payne, K.R. *et al., Ind. Chem.*, 1961, **37**, 523-527 (*manuf, bibl*)
Thies, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1962, **295**, 194-196 (*uv*)
Jerman, L. *et al., Anal. Chim. Acta*, 1966, **36**, 240-241 (*use*)
Carlström, D. *et al., Acta Cryst. B*, 1973, **29**, 161-167 (*cryst struct*)
Hawkins, C.J. *et al., Aust. J. Chem.*, 1973, **26**, 2553-2554 (*resoln*)
Samokish, I.I. *et al., CA*, 1975, **84**, 102283 (*N-Me, isol*)
Nagatsu, T. *et al., Method. Chim.*, 1977, **11**, 194-199 (*rev*)
Szulczewski, D. *et al., Anal. Profiles Drug Subst.*, 1978, **7**, 193-229 (*rev*)
Weisser, U. *et al., Med. Welt*, 1980, **31**, 40-44 (*synth*)
Lai, A. *et al., J.C.S. Faraday 2*, 1981, **77**, 227-233 (*cmr*)
Endress, R. *et al., J. Plant Physiol.*, 1984, **115**, 291-295; *CA*, **101**, 127016u (*occur*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1288 (*synonyms*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **9**, 715-730 (*rev*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 813
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, AES000; VGP000; MJV000; AES250; AES500; EBB500; AES650

Aegeline A-153

N-*[2-Hydroxy-2-(4-methoxyphenyl)ethyl]-3-phenyl-2-propenamide, 9CI.* N-*β-Hydroxy-β-*p-*methoxyphenethylcinnamamide.* N-*Cinnamoyl-2-hydroxy-2-(4-methoxyphenyl)ethylamine. Cinnamic acid 2-hydroxy-2-(*p-*methoxyphenyl)ethylamide. Egeline*
[456-12-2]



$C_{18}H_{19}NO_3$ 297.353
Originally assigned the formula $C_{18}H_{18}O_4$.

(+)-*form* [15298-36-9]
Synthetic. Cryst. (EtOH). Mp 196-197°. $[\alpha]_D^{22}$ +36 (c, 0.4 in $CHCl_3$). $[\alpha]_D^{21}$ -48.1 (c, 0.5 in EtOH).

(-)-*form* [15298-37-0]
Synthetic. Cryst. (EtOH). Mp 196-197°. $[\alpha]_D$ -35.1 ($CHCl_3$). $[\alpha]_D$ +47.5 (c, 0.5 in EtOH).

(±)-*form* [37791-13-2]
Alkaloid from the leaves of *Aegle marmelos* (bael), *Zanthoxylum coriaceum* and *Zanthoxylum ocumarense* (Rutaceae). Antihyperglycaemic and antidyslipidaemic agent. Cryst. (EtOH/EtOAc). Mp 176° (173-175°).

Ac:
$C_{20}H_{21}NO_4$ 339.39
Plates (EtOAc). Mp 124°.

Me ether: N-*[2-Methoxy-2-(4-methoxyphenyl)ethyl]cinnamide. 7-*O-*Methylaegeline*
[70546-93-9]
$C_{19}H_{21}NO_3$ 311.38
Isol. from *Aegle marmelos* (bael). Cryst. (C_6H_6/hexane). Mp 135°. Artifact.

Et ether: N-*[2-Ethoxy-2-(4-methoxyphenyl)ethyl]cinnamide*
[70546-94-0]
$C_{20}H_{23}NO_3$ 325.407
Isol. from *Aegle marmelos* (bael). Cryst. (C_6H_6/hexane). Mp 99-100°. Artifact.

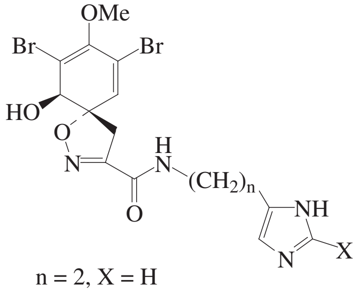
3-Methoxy: ***3-Methoxyaegeline***
$C_{19}H_{21}NO_4$ 327.379
Alkaloid from the leaves of *Zanthoxylum syncarpum*. Cryst. (EtOAc/MeOH). Mp 138-139°. λ_{max} 218 (log ϵ 4.37); 225 (log ϵ 4.57); 278 (log ϵ 4.65) (MeOH).

3-Methoxy, Ac: ***7-*O*-Acetyl-3-methoxyaegeline***
$C_{21}H_{23}NO_5$ 369.416
Alkaloid from the leaves of *Zanthoxylum syncarpum*. Pale yellow powder. λ_{max} 242 (log ϵ 4.82); 252 (log ϵ 4.67); 282 (log ϵ 4.98) (MeOH).

Chatterjee, A. *et al., J.O.C.*, 1959, **24**, 687 (*isol, uv, ir, struct, synth*)
Albónico, S.M. *et al., J.C.S.(C)*, 1967, 1327 (*synth*)
Della Casa de Marcano, D. *et al., Phytochemistry*, 1972, **11**, 1531 (*isol*)
Manandhar, M.D. *et al., Phytochemistry*, 1978, **17**, 1814 (*derivs*)
Patra, A. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 385 (*isol, uv, ir*)
Swinehart, J. *et al., Phytochemistry*, 1980, **19**, 1219 (*isol*)
Patra, A. *et al., Org. Magn. Reson.*, 1981, **16**, 65 (*cmr*)
Sharma, B.R. *et al., Phytochemistry*, 1981, **20**, 2606 (*isol*)
Somanathan, R. *et al., Synth. Commun.*, 1983, **13**, 273 (*synth, ir, ms, pmr, cmr*)
Brown, R.F.C. *et al., Tetrahedron: Asymmetry*, 1993, **4**, 205 (*synth*)
Ross, S.A. *et al., J. Nat. Prod.*, 2005, **68**, 1297-1299 (*3-Methoxyaegeline, 7-Acetyl-3-methoxyaegeline*)
Narender, T. *et al., Bioorg. Med. Chem. Lett.*, 2007, **17**, 1808-1811 (*isol, activity*)

Aerophobin 1 A-154

[87075-24-9]



$C_{15}H_{16}Br_2N_4O_4$ 476.124
Isol. from the sponges *Verongia aerophoba* and *Verongula rigida*. Also from *Tylodina perversa*. Mp 164-167° (Ac). $[\alpha]_D$ +187 (c, 2.0 in MeOH).

Cimino, G. *et al., Tet. Lett.*, 1983, **24**, 3029 (*isol, pmr, cmr, ms, struct*)
Nishiyama, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 3453 (*synth*)
Gunasekera, M. *et al., J. Nat. Prod.*, 1989, **52**, 753 (*isol, uv, ir, pmr, cmr, ms*)
Teeyapant, R. *et al., Z. Naturforsch., C*, 1993, **48**, 640-644 (*isol*)

Aerophobin 2 A-155

[87075-23-8]
As Aerophobin 1, A-154 with
n = 3, X = NH_2
$C_{16}H_{19}Br_2N_5O_4$ 505.165
Isol. from the sponges *Verongia aerophoba* and *Aiolochroia crassa*. $[\alpha]_D$ +139 (c, 1.9 in MeOH).

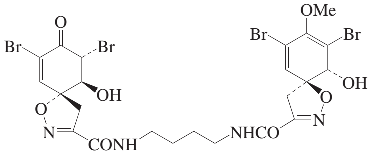
N-*Me (X = NHMe)*: **N-*Methylaerophobin 2***
[209472-96-8]
$C_{17}H_{21}Br_2N_5O_4$ 519.192
Alkaloid from the sponge *Aiolochroia crassa*.

13,14-Dihydro, 14-oxo: ***14-Oxoaerophobin 2***
[232259-26-6]
$C_{16}H_{19}Br_2N_5O_5$ 521.165
Isol. from *Aplysina insularis*.

Cimino, G. *et al., Tet. Lett.*, 1983, **24**, 3029 (*Aerophobin 2*)
Assmann, M. *et al., Z. Naturforsch., C*, 1998, **53**, 398-401 (*N-Methylaerophobin 2*)
Fendert, T. *et al., Z. Naturforsch., C*, 1999, **54**, 246-251 (*14-Oxoaerophobin 2*)

Aeroplysinillin A-156

[1056030-28-4]



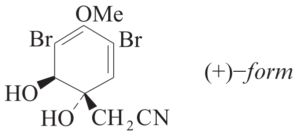
Relative Configuration

$C_{23}H_{24}Br_4N_4O_8$ 804.081
Closely related to Aerothionin, A-158. Isol. from an *Aplysinella* sp. Powder. $[\alpha]_D^{20}$ +38.2 (c, 0.2 in MeOH). λ_{max} 223 (log ε 5.5); 256 (log ε 5.48) (MeOH).

Ankudey, F.J. *et al., Planta Med.*, 2008, **74**, 555-559 (*isol, cd, pmr, cmr*)

Aeroplysinin 1 A-157

3,5-Dibromo-1,6-dihydroxy-4-methoxy-2,4-cyclohexadiene-1-acetonitrile, 9CI. 3,5-Dibromo-1-cyanomethyl-4-methoxy-3,5-cyclohexadiene-1,2-diol. Zamamistatin



$C_9H_9Br_2NO_3$ 338.983
Structure of Zamamistatin revised twice; finally shown to be the same as Aeroplysinin 1 in 2008.

(+)-form [28656-91-9]
Constit. of the sponges *Aplysina aerophoba (Verongia aerophoba)*, *Aplysina archeri*, *Aiolochroia crassa*, *Verongula rigida*, *Psammaplysilla purpurea*, *Ianthella* sp. and others. Cytotoxic and antibacterial agent. Protein-tyrosine kinase inhibitor. Algicide, molluscicide. Sol. MeOH, Et_2O, Me_2CO; poorly sol. hexane. Mp 120-121° (112-113°). $[\alpha]_D$ +193 (c, 0.63 in Me_2CO). $[\alpha]_D^{20}$ +185 (c, 0.17 in MeOH). λ_{max} 284 (ε 4910) (MeOH) (Derep). λ_{max} 231 (ε 3220); 284 (ε 4910) (MeOH) (Berdy).
▶ GU4735000

Di-Ac:
Cryst. (C_6H_6/petrol). Mp 114°. $[\alpha]_D$ +218 ($CHCl_3$).

(-)-form
Constit. of the sponges *Ianthella ardis*, *Verongula gigantea*, *Suberea creba*, *Psammaplysilla arabica* and *Pseudoceratina crassa*. Mp 116-117°. $[\alpha]_D^{20}$ -176 (c, 0.125 in MeOH). $[\alpha]_D$ -198 (c, 0.5 in Me_2CO). λ_{max} 284 (ε 4910) (MeOH) (Derep).

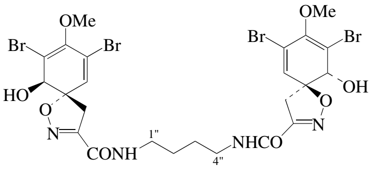
(±)-*form*
Constit. of *Verongula gigantea* and *Aiolochroia crassa*. Mp 153-154°. λ_{max} 284 (ε 4910) (MeOH) (Derep).

[55057-73-3 , 55057-74-4 , 66141-25-1 , 30951-40-7]

Fulmor, W. *et al., Tet. Lett.*, 1970, 4551 (*ir, pmr, cd, abs config*)
Cosulich, D.B. *et al., Chem. Comm.*, 1971, 397 (*cryst struct, abs config*)
Mazzarella, L. *et al., Gazz. Chim. Ital.*, 1972, **102**, 391 (*cryst struct, abs config*)
Fattorusso, E. *et al., J.C.S. Perkin 1*, 1972, 16 (*isol, uv, ir, pmr, ms, struct*)
Andersen, R.J. *et al., J.A.C.S.*, 1975, **97**, 936 (*synth*)
Chang, C.W.J. *et al., Tet. Lett.*, 1977, 4005 (*isol*)
Makarieva, T.N. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1981, **68**, 481 (*isol, uv, ir, ms*)
Koulman, A. *et al., J. Nat. Prod.*, 1996, **59**, 591 (*activity*)
Kita, M. *et al., Tet. Lett.*, 2008, **49**, 5383-5384 (*Zamamistatin*)

Aerothionin A-158

[28714-26-3]



$C_{24}H_{26}Br_4N_4O_8$ 818.107
Numbering systems vary. Isol. from *Aplysina aerophoba* (*Verongia aerophoba*), *Aplysina fistularis* and *Aplysina thiona*. Also from *Pseudoceratina durissima*, *Psammaplysilla purpurea* and the crinoid *Himerometra magnipinna*. Plates (Me_2CO/C_6H_6). Mp 134-137° dec. $[\alpha]_D$ +252 (Me_2CO). λ_{max} 234 (ε 14450); 284 (ε 13490) (EtOH) (Derep). λ_{max} 284 (ε 12660) (MeOH) (Berdy).

Di-Ac:
Needles (Me_2CO). Mp 206-208°. $[\alpha]_D$ +236 ($CHCl_3$).

2″-Hydroxy: ***11-Hydroxyaerothionin***
[73622-27-2]
$C_{24}H_{26}Br_4N_4O_9$ 834.107
Constit. of *Aplysina caissara*, *Aplysina lacunosa* and *Pseudoceratina durissima*. Glass. $[\alpha]_D$ +189 (c, 0.15 in MeOH). λ_{max} 233 (ε 19780); 284 (ε 11100); 295 (ε 18900) (MeOH) (Berdy).

2″,3″-Dihydroxy: ***Dihydroxyaerothionin***
[122759-72-2]
$C_{24}H_{26}Br_4N_4O_{10}$ 850.106
Metab. of *Verongula rigida*. Powder. Mp 162-164°. $[\alpha]_D^{25}$ -64.2 (c, 0.1 in MeOH).

2″-Oxo: ***11-Oxoaerothionin***
[73622-23-8]
$C_{24}H_{24}Br_4N_4O_9$ 832.091
Metab. from the Caribbean sponge *Aplysina lacunosa* and from *Verongia cavernicola*. Exhibits pronounced and selective antitumour activity against human colon (HCT116) cell line. Powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 174.6-176.6° dec. $[\alpha]_D^{25}$ +181.15 (c, 2.17 in DMSO). λ_{max} 262 (ε 11600); 284 (ε 11500) (MeOH) (Berdy).

*2″-Oxo, 3″*R*-hydroxy*: ***12*R*-Hydroxy-11-oxoaerothionin***
[157544-68-8]
$C_{24}H_{24}Br_4N_4O_{10}$ 848.09
Metab. from the Caribbean sponge *Aplysina fistularis* forma *fulva*. $[\alpha]_D^{25}$ +160.7.

*2″-Oxo, 3″*S*-hydroxy*: ***12*S*-Hydroxy-11-oxoaerothionin***
[157497-57-9]
$C_{24}H_{24}Br_4N_4O_{10}$ 848.09
Metab. from the sponge *Aplysina fistularis* forma *fulva*. $[\alpha]_D^{25}$ +152.5.

Homologue: ***Homoaerothionin***
[34232-66-1]
[35036-48-7]
$C_{25}H_{28}Br_4N_4O_8$ 832.134
Constit. of the sponges *Aplysina aerophoba*, *Verongia thiona* and *Verongia cavernicola*. Amorph. solid. Mp 166-167° (as di-Ac). $[\alpha]_D$ +191.5 ($CHCl_3$) (di-Ac). Has a C_5 bridging chain instead of C_4. λ_{max} 289 (ε 13348) (MeOH) (Berdy).

Homologue, 2″ξ-hydroxy: 11-Hydroxyhomoaerothionin. ***Caissarine C***
$C_{25}H_{28}Br_4N_4O_9$ 848.134
Constit. of *Aplysina caissara*. Amorph. solid. $[\alpha]_D^{28}$ +175 (c, 0.002 in MeOH).

Homologue, 3″-hydroxy: ***12-Hydroxyhomoaerothionin***
[938464-19-8]
$C_{25}H_{28}Br_4N_4O_9$ 848.134
Isol. from the crinoid *Himerometra magnipinna*. Yellow powder. $[\alpha]_D^{20}$ +106 (c, 0.39 in MeOH). λ_{max} 231 (log ε 4.33); 281 (log ε 3.99) (MeOH).

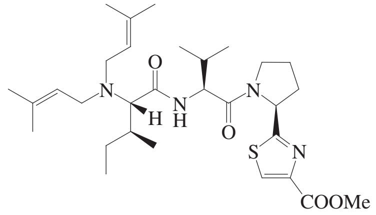
Homologue, 2″-oxo: ***11-Oxohomoaerothionin***
[191112-17-1]
$C_{25}H_{26}Br_4N_4O_9$ 846.118
Constit. of *Aplysina cavernicola*. λ_{max} 232 (ε 19000); 284 (10500) (MeOH).

Fattorusso, E. *et al., Chem. Comm.*, 1970, 752-753 (*uv, ir, pmr, struct*)
Fattorusso, E. *et al., Gazz. Chim. Ital.*, 1971, **101**, 61-63 (*Homoaerothionin*)
Moody, K. *et al., J.C.S. Perkin 1*, 1972, 18-24 (*isol, uv, ir, pmr, struct, Homoaerothionin*)
Forrester, A.R. *et al., Annalen*, 1978, 66-73 (*synth*)

McMillan, J.A. *et al., Tet. Lett.*, 1981, **22**, 39-42 (*cryst struct, uv, pmr, cd, abs config*)
Nishiyama, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 3453-3456 (*synth*)
Okamoto, K.T. *et al., Tet. Lett.*, 1987, **28**, 4969-4972 (*biosynth*)
Gunasekera, M. *et al., J. Nat. Prod.*, 1989, **52**, 753-756 (*Dihydroxyaerothionin*)
Kernan, M.R. *et al., J. Nat. Prod.*, 1990, **53**, 615-622 (*11-Hydroxyaerothionin*)
Acosta, A.L. *et al., J. Nat. Prod.*, 1992, **55**, 1007-1012 (*11-Oxoaerothionin*)
Ciminiello, P. *et al., J. Nat. Prod.*, 1994, **57**, 705-712 (*12-Hydroxy-11-oxoaerothionin*)
Ciminiello, P. *et al., Tetrahedron*, 1997, **53**, 6565-6572 (*11-Oxohomoaerothionin*)
Wasserman, H.H. *et al., J.O.C.*, 1998, **63**, 5581-5586 (*synth*)
De Lira, T.O. *et al., J. Braz. Chem. Soc.*, 2006, **17**, 1233-1240 (*Caissarine C*)
Ogamino, T. *et al., Tet. Lett.*, 2006, **47**, 727-731 (*synth, abs config*)
Shao, N. *et al., J. Nat. Prod.*, 2007, **70**, 869-871 (*12-Hydroxyhomoaerothionin*)

Aeruginosamide A-159

[241483-64-7]



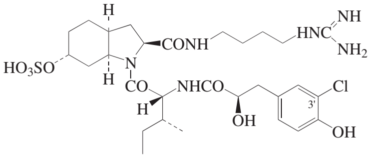
$C_{30}H_{48}N_4O_4S$ 560.8

Modified peptide antibiotic. Isol. from *Microcystis aeruginosa*. Moderate cytotoxic agent. Pale green oil. $[\alpha]_D$ -71.4 (c, 0.01 in $CHCl_3$).

Lawton, L.A. *et al., J.O.C.*, 1999, **64**, 5329-5332 (*isol, pmr, cmr, ir, ms*)
Chen, Z. *et al., New J. Chem.*, 2006, **30**, 518-520 (*synth*)

Aeruginosin 98A A-160

[167172-80-7]



Absolute Configuration

$C_{29}H_{45}ClN_6O_9S$ 689.228

Isol. from the blue-green alga *Microcystis aeruginosa* NIES98. Inhibitor of trypsin, thrombin and serine proteases. Amorph. powder. Sol. MeOH, H_2O. $[\alpha]_D$ -7.6 (c, 0.2 in H_2O). λ_{max} 279 (ϵ 1472) (H_2O) (Berdy).

5′-Chloro: ***Aeruginosin 101***
$C_{29}H_{44}Cl_2N_6O_9S$ 723.673
Isol. from *Microcystis aeruginosa*. Protease inhibitor. $[\alpha]_D$ -11 (c, 0.5 in MeOH aq.). λ_{max} 290 (ϵ 1810) (MeOH).

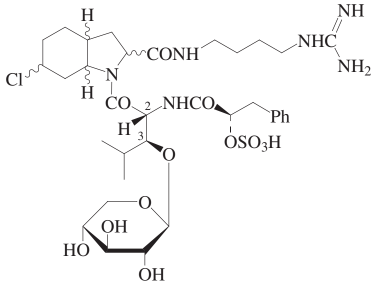
3′-Dechloro: ***Aeruginosin 98B***
[167228-01-5]
$C_{29}H_{46}N_6O_9S$ 654.783
Isol. from *Microcystis aeruginosa* NIES98. Inhibitor of trypsin, thrombin, plasmin and serine proteases. Amorph. powder. Sol. MeOH, H_2O. $[\alpha]_D$ -5.2 (c, 0.2 in H_2O). λ_{max} 276 (ϵ 1177) (H_2O) (Berdy).

3′-Dechloro, 3′-bromo: ***Aeruginosin 98C***
[167172-73-8]
$C_{29}H_{45}BrN_6O_9S$ 733.679
Isol. from *Microcystis aeruginosa* NIES98. Serine protease inhibitor. Powder. Sol. MeOH, H_2O. $[\alpha]_D$ -13 (c, 0.25 in H_2O). λ_{max} 281 (ϵ 860) (H_2O).

Murakami, M. *et al., Tet. Lett.*, 1995, **36**, 2785-2788 (*isol, pmr, cmr*)
Ishida, K. *et al., Tetrahedron*, 1999, **55**, 10971-10988 (*isol, abs config*)
Ersmark, K. *et al., Angew. Chem., Int. Ed.*, 2008, **47**, 1202-1223 (*rev*)

Aeruginosin 205A A-161

[184015-81-4]



$C_{34}H_{53}ClN_6O_{12}S$ 805.344

Glycopeptide antibiotic. Structure probably requires revision. Isol. from freshwater *Oscillatoria agardhii* NIES 205. Serine protease inhibitor. Microcryst. Sol. MeOH, butanol; fairly sol. H_2O; poorly sol. Et_2O, hexane. $[\alpha]_D^{20}$ +17.7 (c, 0.1 in MeOH). λ_{max} 258 (ϵ 520) (MeOH).

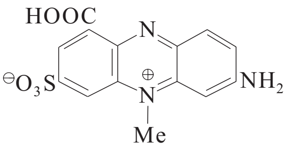
2,2′,3-Triepimer: ***Aeruginosin 205B***
[187521-09-1]
$C_{34}H_{53}ClN_6O_{12}S$ 805.344
Isol. from freshwater *Oscillatoria agardhii* NIES 205. Serine protease inhibitor. Sol. MeOH, butanol; fairly sol. H_2O; poorly sol. Et_2O, hexane. $[\alpha]_D^{20}$ +40.3 (c, 0.1 in MeOH). λ_{max} 258 (ϵ 570) (MeOH).

Shin, H.J. *et al., J.O.C.*, 1997, **62**, 1810-1813 (*isol, uv, pmr, cmr, ms*)
Valls, N. *et al., Tet. Lett.*, 2006, **47**, 3701-3705 (*struct*)
Ersmark, K. *et al., Angew. Chem., Int. Ed.*, 2008, **47**, 1202-1223 (*rev*)

Aeruginosin B A-162

7-Amino-1-carboxy-5-methyl-3-sulfophenazinium hydroxide inner salt, 9CI. 7-Amino-1-carboxy-5-methyl-3-sulfophenazinium betaine. Eruginosin B

[6508-65-2]



$C_{14}H_{11}N_3O_5S$ 333.324

Pigment from *Pseudomonas aeruginosa*. Red cryst. (aq. acid). Sol. H_2O. Dec. on heating without melting.

Herbert, R.B. *et al., J.C.S.(C)*, 1969, 2517 (*struct, ir, uv*)
Bentley, R.K. *et al., J.C.S.(C)*, 1970, 2447 (*synth*)

Aestivine† A-163

Estivine

[1356-93-0]

Struct. unknown

$C_{17}H_{21}NO_4$ 303.357

Amaryllidaceae alkaloid. Isol. from the bulbs of *Leucojum aestivum* (Amaryllidaceae). Cryst. + $1H_2O$ (EtOH). Mp 194-195°. $[\alpha]_D$ -151 (c, 0.1 in EtOH).

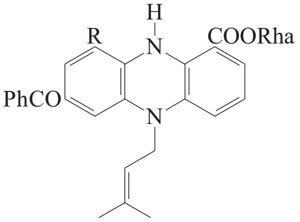
Hydrochloride:
Cryst. + ½ H_2O. Mp 205-207°.

Hydrobromide: Mp 153-154°.

Proskurnina, N.F. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1963, **33**, 1643-1644 (*isol*)

Aestivophoenin A A-164

[171864-91-8]



R = H

$C_{31}H_{32}N_2O_7$ 544.603

Phenazine antibiotic. Prod. by *Streptomyces purpeofuscus.* Neuronal cell protecting agent, neuroprotectant, lipid peroxidation inhibitor. Orange powder. Sol. MeOH, EtOAc, Me_2CO. Mp 59-61°. $[\alpha]_D^{20}$ -106.3 (c, 0.005 in MeOH). λ_{max} 229 (ϵ 28900); 245 (ϵ 27400); 296 (ϵ 26000); 367 (ϵ 4000); 490 (ϵ 11700) (MeOH) (Berdy).

Shin-ya, K. *et al., J. Antibiot.*, 1995, **48**, 1378 (*isol, pmr, cmr, uv, ir*)

Aestivophoenin B A-165

[171864-92-9]

As Aestivophoenin A, A-164 with

R = $-CH_2CH{=}C(CH_3)_2$

$C_{36}H_{40}N_2O_7$ 612.721

Phenazine antibiotic. Prod. by *Streptomyces purpeofuscus.* Neuronal cell protecting agent, neuroprotecant, lipid peroxidation inhibitor. Orange powder. Sol. MeOH, Me_2CO, EtOAc. Mp 63-64°. $[\alpha]_D$ -139.8 (c, 0.006 in MeOH). λ_{max} 232 (ϵ 26900); 245 (ϵ 25800); 298 (ϵ 19000); 368 (ϵ 3300); 495 (ϵ 9700) (MeOH) (Berdy).

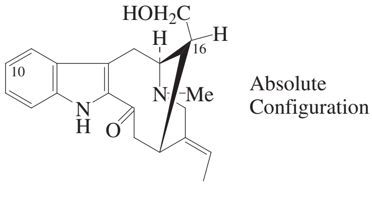
Debenzoyl: ***Aestivophoenin C***
$C_{29}H_{36}N_2O_6$ 508.613
Prod. by *Streptomyces purpeofuscus.* Neuronal cell protecting agent, antioxidant. Yellow powder. Mp 61-62°.

λ_{max} 247 (ϵ 24600); 328 (ϵ 2000); 453 (ϵ 4100) (MeOH).

Shin-ya, K. *et al., J. Antibiot.*, 1995, **48**, 1378 (*isol, pmr, cmr, uv, ir*)
Kunigami, T. *et al., J. Antibiot.*, 1998, **51**, 880-882 (*isol, uv, pmr, cmr*)

Affinine† A-166

17-Hydroxyvobasan-3-one, 9CI
[2134-82-9]



$C_{20}H_{24}N_2O_2$ 324.422
Alkaloid from *Peschiera affinis*, *Peschiera laeta* and *Tabernaemontana psychotrifolia* (Apocynaceae). Cryst. (MeOH/EtOAc, CH_2Cl_2/heptane, or EtOH). Mp 273-275° (264-265°) dec. $[\alpha]_D^{24}$ -180 (c, 0.78 in EtOH). λ_{max} 236 (sh) (ϵ 13200); 320 (ϵ 13400) (EtOH).

Hydrochloride:
Cryst. (MeOH/EtOAc). Mp 267-269° dec. $[\alpha]_D^{25}$ -105.4 (c, 0.5 in MeOH).

O-*Ac:*
Cryst. as solvate (Me_2CO). Mp 95-115°.

10-Methoxy: ***Pelirine***
[30435-26-8]
$C_{21}H_{26}N_2O_3$ 354.448
Alkaloid from the roots of *Rauwolfia perakensis* (Apocynaceae). Pale yellow plates (MeOH aq.). Mp 130-131°. $[\alpha]_D^{22}$ -121 (c, 1 in EtOH). The 16-config. was uncertain until 1987.

10-Methoxy, sulfate (1:2):
Cryst. + ½ H_2O. Mp 223-224° dec.

10-Methoxy, picrate:
Yellow needles (EtOH). Mp 159-159.5°.

16-Epimer: ***16-Epiaffinine***
[38990-09-9]
$C_{20}H_{24}N_2O_2$ 324.422
Alkaloid from the stem bark of *Pleiocarpa talbotii* (Apocynaceae). Cryst. (Et_2O/pentane). Mp 152-154°. $[\alpha]_D^{23}$ -190 (c, 0.95 in $CHCl_3$). pK_a 6.9 (methylcellosolve).

16-Epimer, picrate:
Cryst. (MeOH). Mp 187-189°.

16-Epimer, N-*Me:* ***16-Epi-*N*-methylaffinine***. N-*Methyl-16-epiaffinine*
[58262-66-1]
$C_{21}H_{26}N_2O_2$ 338.449
Alkaloid from *Tabernaemontana accedens* (Apocynaceae). Plates (MeOH). Mp 208-210° dec. $[\alpha]_D^{20}$ -243 (c, 0.05 in $CHCl_3$).

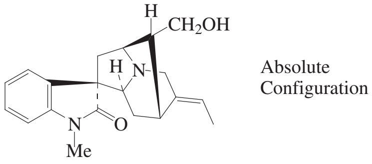
16-Epimer, Me ether: **Hystrixnine**. *16-Epi-17-*O*-methylaffinine*
$C_{21}H_{26}N_2O_2$ 338.449
Alkaloid from the root bark of *Tabernaemontana hystrix*. Amorph. solid. $[\alpha]_D^{25}$ -100 (c, 0.66 in MeOH). λ_{max} 223 (ϵ 42570); 282 (ϵ 6290) (MeOH).

16-Epimer, 10-hydroxy: ***16-Epi-10-hydroxyaffinine***. *10-Hydroxy-16-epiaffinine*
[82513-70-0]
$C_{20}H_{24}N_2O_3$ 340.421
Alkaloid from *Hunteria zeylanica* (Apocynaceae). Amorph. $[\alpha]_D$ -122 (c, 0.46 in $CHCl_3$). λ_{max} 212 (log ϵ 4.46); 228 (sh) (log ϵ 4.29); 277 (sh) ; 328 (log ϵ 4.17) (MeOH).

Kiang, A.K. *et al., J.C.S.*, 1960, 1394-1398 (*Pelirine, isol, uv*)
Weisbach, J.A. *et al., J. Pharm. Sci.*, 1963, **52**, 350-353 (*isol, ir*)
Cava, M.P. *et al., Chem. Ind. (London)*, 1964, 1193-1194 (*struct, pmr*)
Burnell, R.H. *et al., Can. J. Chem.*, 1971, **49**, 307-316 (*isol, uv, ir, pmr, struct*)
Naranjo, J. *et al., Helv. Chim. Acta*, 1972, **55**, 752-771 (*16-Epiaffinine*)
Bláha, K. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 929-933 (*Pelirine, cd*)
Achenbach, H. *et al., Chem. Ber.*, 1975, **108**, 3842-3854 (*16-Epi-N-methylaffinine*)
Voticky, Z. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 1403-1406 (*isol, uv, ir, ms*)
Lavaud, C. *et al., Phytochemistry*, 1982, **21**, 445-447 (*16-Epi-10-hydroxyaffinine*)
Wan, A.S.C. *et al., Heterocycles*, 1987, **26**, 1211-1214 (*Pelirine, cryst struct, abs config*)
Monnerat, C.S. *et al., J. Braz. Chem. Soc.*, 2005, **16**, 1331-1335 (*Hystrixnine*)

Affinisine oxindole A-167

[701950-31-4]

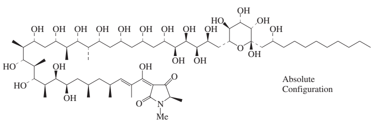


$C_{20}H_{24}N_2O_2$ 324.422
Alkaloid from the leaves of *Alstonia angustifolia* var. *latifolia*. Light yellow oil. $[\alpha]_D$ -70 (c, 0.06 in $CHCl_3$). λ_{max} 211 (log ϵ 4.31); 233 (log ϵ 3.82); 255 (log ϵ 3.87); 290 (log ϵ 3.35) (EtOH).

Kam, T.-S. *et al., Phytochemistry*, 2004, **65**, 603-608 (*isol, pmr, cmr*)

Aflastatin A A-168

[179729-59-0]



$C_{62}H_{115}NO_{24}$ 1258.583
Abs. config. revised in 2007. Prod. by *Streptomyces* sp. MRI 142. Inhibits production of Aflatoxin by aflatoxigenic fungi. Active against *Candida*, *Trichophyton* and *Staphylococcus* infections. Powder. Sol. DMSO; fairly sol. MeOH; poorly sol. H_2O, $CHCl_3$, hexane, EtOAc, Me_2CO. $[\alpha]_D^{19}$ -2.6 (c, 0.5 in DMSO). λ_{max} 247 (ϵ 11000); 299 (ϵ 6200) (MeOH aq.). λ_{max} 237 (ϵ 7900); 314 (ϵ 7300) (MeOH/HCl). λ_{max} 247 (ϵ 11000); 299 (ϵ 6200) (MeOH/NaOH).

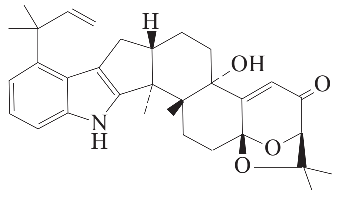
▶ LD_{50} (mus, ipr) 6.17 mg/kg, LD_{50} (mus, orl) 2000 mg/kg.

N-*De-Me:* ***Aflastatin B***
$C_{61}H_{113}NO_{24}$ 1244.556
Prod. by *Streptomyces* MRI142. $[\alpha]_D^{23}$ -0.6 (c, 0.16 in DMSO). λ_{max} 246 (ϵ 10600); 299 (ϵ 6300) (MeOH aq.). λ_{max} 237 (ϵ 8000); 314 (ϵ 7800) (MeOH/HCl). λ_{max} 299 (ϵ 6300) (MeOH/NaOH).

Sakuda, S. *et al., J.A.C.S.*, 1996, **118**, 7855-7856 (*biosynth, struct*)
Ono, M. *et al., J. Antibiot.*, 1997, **50**, 111-118; 1998, **51**, 1019-1029 (*isol, uv, ir, pmr, cmr, props, ms*)
Ikeda, H. *et al., J.O.C.*, 2000, **65**, 438-444 (*abs config*)
Sakuda, S. *et al., Tet. Lett.*, 2007, **48**, 2527-2531 (*abs config*)

Aflatrem A-169

α,α-Dimethylallylpaspalinine
[70553-75-2]



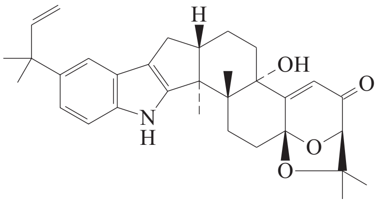
$C_{32}H_{39}NO_4$ 501.664
Isol. from *Aspergillus flavus* and *Claviceps paspali*. Tremorgenic mycotoxin. Needles (Me_2CO/Et_2O). Sol. MeOH, $CHCl_3$. Mp 222-224°. λ_{max} 231 (ϵ 27700); 250 (ϵ 10000); 282 (ϵ 9000) (MeOH) (Berdy).

▶ Toxic.

Wilson, B.J. *et al., Science (Washington, D.C.)*, 1964, **144**, 177 (*isol*)
Gallagher, R.T. *et al., Tet. Lett.*, 1980, 239 (*struct, uv, ir, pmr, cmr*)
Cole, R.J. *et al., J. Agric. Food Chem.*, 1981, **29**, 293 (*isol*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 410

Aflatrem B A-170

β-Aflatrem
[144446-23-1]

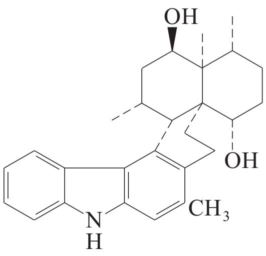


$C_{32}H_{39}NO_4$ 501.664
Prod. by *Aspergillus flavus*, *Aspergillus parasiticus* and *Aspergillus subolivaceus*. Mycotoxin, exhibits insecticidal activity. Yellow cryst. Mp 188-190°. $[\alpha]_D$ +77.9 (c, 0.011 in $CHCl_3$). λ_{max} 233 (ϵ 18500); 264 (ϵ 6300); 296 (ϵ 2700) (MeOH) (Berdy).

TePaske, M.R. *et al., J. Nat. Prod.*, 1992, **55**, 1080 (*isol, uv, pmr, cmr, ms, struct*)

Aflavazole A-171

[133401-09-9]



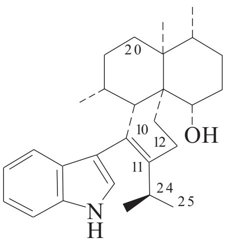
$C_{28}H_{35}NO_2$ 417.59

Closely related to Aflavinine, A-172. Metab. of *Aspergillus flavus* and *Aspergillus parasiticus.* Exhibits pronounced insect antifeedant activity. Light yellow cryst. Mp 156-160° dec. $[\alpha]_D$ +2.8 (c, 0.35 in MeOH). λ_{max} 219 (ϵ 15300); 243 (ϵ 17300); 263 (ϵ 7500); 297 (ϵ 7600); 327 (ϵ 1300); 341 (ϵ 1600) (MeOH) (Derep).

TePaske, M.R. *et al., J.O.C.*, 1990, **55**, 5299 (*isol, pmr, cmr*)

Aflavinine A-172

[74328-59-9]



$C_{28}H_{39}NO$ 405.622

Indolic diterpenoid antibiotic. Related to biosynthetic intermeds. in the penitrem series. Differnt numbering systems in use. Isol. from *Aspergillus flavus*, *Eupenicillium crustaceum* and *Eupenicillium molle.* Tremorgenic mycotoxin, shows insecticidal activity. Needles + 1EtOAc (EtOAc). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 102-104°. λ_{max} 226 (ϵ 27000); 284 (ϵ 5300); 292 (ϵ 4500) (MeOH) (Berdy).

10β,11α-Dihydro, 24,25-didehydro: 24,25-Dehydro-10,11-dihydroaflavinine
[124693-66-9]
$C_{28}H_{39}NO$ 405.622
Metab. from the sclerotia of *Aspergillus tubingensis.* Also shown by hplc to be present in the sclerotia of *Aspergillus flavus* and *Aspergillus parasiticus.* Mp 192-194°. $[\alpha]_D$ -1.2 (c, 0.5 in $CHCl_3$).

20β-Hydroxy: ***20-Hydroxyaflavinine***
[116865-08-8]
$C_{28}H_{39}NO_2$ 421.622
From *Aspergillus flavus.* Tremorgenic mycotoxin, shows antifeedant and insecticidal props. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 174-176° dec. (161-162°). $[\alpha]_D$ +64 (c, 0.08 in MeOH). $[\alpha]_D$ +23.8 (c, 0.56 in MeOH). λ_{max} 224 (ϵ 14900); 283 (ϵ 2760); 290 (ϵ 2520) (MeOH) (Derep).

20α-Hydroxy, 10β,11α-dihydro, 24,25-didehydro: ***24,25-Dehydro-10,11-dihydro-20-epi-20-hydroxyaflavinine***
$C_{28}H_{39}NO_2$ 421.622
Metab. from the sclerotia of *Aspergillus tubingensis.* Also shown by hplc to be present in the sclerotia of *Aspergillus flavus* and *Aspergillus parasiticus.* Mp 79-82°. $[\alpha]_D$ -5.6 (c, 1.06 in $CHCl_3$). λ_{max} 226 (ϵ 16400); 284 (ϵ 2290); 292 (ϵ 2100) (MeOH) (Berdy).

20β-Hydroxy, 10β,11α-dihydro, 11,12-didehydro: ***11,12-Didehydro-10,11-dihydro-20-hydroxyaflavinine***
[116865-10-2]
$C_{28}H_{39}NO_2$ 421.622
From *Aspergillus flavus.* Mycotoxin showing insecticidal and antifeedant props. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 276-278°. $[\alpha]_D$ +1.7 (c, 0.1 in MeOH). λ_{max} 224 (ϵ 20030); 281 (ϵ 3600); 285 (ϵ 3380) (MeOH) (Berdy).

20β-Hydroxy, 10β,11α-dihydro, 24,25-didehydro: ***24,25-Dehydro-10,11-dihydro-20-hydroxyaflavinine****. Monohydroxyisoaflavinine*
$C_{28}H_{39}NO_2$ 421.622
Metab. from *Aspergillus flavus.* insecticide, tremorigenic agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 146-148° Mp 259-262°. $[\alpha]_D$ +0.9 (c, 0.34 in MeOH). $[\alpha]_D^{24}$ +56 (c, 0.10 in MeOH). Identical structs. assigned to Dehydrodihydro-20-hydroxyaflavinine and Monohydroxyisoaflavinine (Nozawa *et al*) but very different props. reported (lower Mp and higher opt. rotn. refer to Monohydroxyisoaflavinine). λ_{max} 226 ; 227 (ϵ 26260); 284 (ϵ 6060); 291 (ϵ 5220) (MeOH) (Berdy). λ_{max} 226 (ϵ 21380); 283 (ϵ 4266); 291 (ϵ 3990) (EtOH) (Berdy).

24-Hydroxy, 10,11-dihydro: ***10,11-Dihydro-24-hydroxyaflavinine***
[171569-81-6]
$C_{28}H_{41}NO_2$ 423.637
Prod. by *Eupenicillium crustaceum.* Shows insecticidal props. Powder. $[\alpha]_D$ -22 ($CHCl_3$).

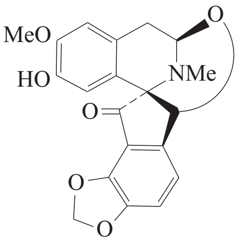
20β,25-Dihydroxy: ***20,25-Dihydroxyaflavinine***
[76410-56-5]
$C_{28}H_{39}NO_3$ 437.621
From *Aspergillus flavus.* Tremorgenic mycotoxin, shows insecticidal and antifeedant props. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 254-256°. $[\alpha]_D$ +22.9 (c, 0.5 in MeOH). λ_{max} 224 (ϵ 20190); 283 (ϵ 3850); 291 (ϵ 3670) (MeOH) (Berdy).

13-Oxo, 10β,11α-dihydro, 24,25-didehydro: ***24,25-Dehydro-10,11-dihydro-13-oxoaflavinine***
[124693-67-0]
$C_{28}H_{37}NO_2$ 419.606
From *Aspergillus tubingensis.* Shows insecticidal props. Mp 138-141°. $[\alpha]_D$ -13.5 (c, 0.72 in $CHCl_3$). λ_{max} 224 (ϵ 18200); 267 (ϵ 1200); 273 (ϵ 1400); 283 (ϵ 2100); 291 (ϵ 1750) (MeOH) (Berdy).

Gallagher, R.T. *et al., Tet. Lett.*, 1980, 243 (*isol, pmr, cmr, cryst struct*)
Cole, R.J. *et al., J. Agric. Food Chem.*, 1981, **29**, 293 (*deriv*)
Danishefsky, S. *et al., J.A.C.S.*, 1985, **107**, 2474 (*synth*)
Gloer, J.B. *et al., J.O.C.*, 1988, **53**, 5457 (*isol, derivs*)
Nozawa, K. *et al., Chem. Pharm. Bull.*, 1989, **37**, 626 (*Monohydroxyisoaflavinine, isol, uv, pmr, cmr, ms, cryst struct*)
TePaske, M.R. *et al., Tetrahedron*, 1989, **45**, 4961 (*derivs*)
Wang, H.J. *et al., Appl. Environ. Microbiol.*, 1995, **61**, 4429-4435 (*10,13-Dihydro-24-hydroxyaflavinine*)

Africanine A-173

[107019-97-6]



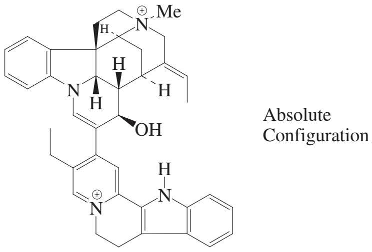
$C_{20}H_{17}NO_6$ 367.357

Alkaloid from *Rupicapnos africana* (Papaveraceae). Cryst. (MeOH). Mp 237°. $[\alpha]_D^{25}$ +22 (c, 0.322 in $CHCl_3$).

Castedo, L. *et al., Heterocycles*, 1986, **24**, 2781 (*uv, ir, pmr, ms, struct*)

Afrocurarine A-174

[55599-19-4]



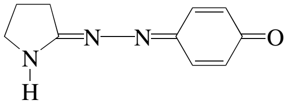
$C_{39}H_{42}N_4O^{2\oplus}$ 582.787

Alkaloid from *Strychnos usambarensis* (Loganiaceae). Weak neuromuscular blocking agent (activity *ca.* 0.05 × Tubocurarine).

Caprasse, M. *et al., Planta Med.*, 1984, **50**, 131-133 (*isol, uv, ir, pmr, ms, cd, struct*)

Agaricone A-175

[99280-73-6]



$C_{10}H_{11}N_3O$ 189.216

Isol. from the toadstool *Agaricus xanthoderma.* Red cryst. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 115° (dec.).

Formed on injury of the fungus by air or enzyme oxidn. of Leucoagaricone, L-154. λ_{max} 242 (log ϵ 3.74); 427 (log ϵ 4.19) (MeOH).

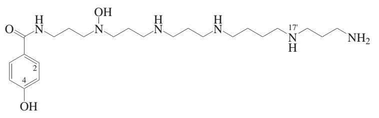
Hilbig, S. *et al., Angew. Chem., Int. Ed.*, 1985, **24**, 1063-1065 (*isol, synth, uv, pmr, ms*)

Agel 452 A-176

N-*(20-Amino-4-hydroxy-4,8,12,17-tetraazaeicos-1-yl)-4-hydroxybenzamide, 9CI. AG 452*

[128549-98-4]

[128550-23-2 (trifluoroacetate salt)]



$C_{23}H_{44}N_6O_3$ 452.639

See also *Agelenopsis aperta* Hydroxybenzoylpentamine toxins, H-413 for related toxins. Alkaloid from the venom of the spider *Agelenopsis aperta*. λ_{max} 251 (log ϵ 4.12) (H_2O) (trifluoroacetate).

4-Deoxy, 2,5-dihydroxy: ***Agel 468****. AG 468*
[128549-99-5]
$C_{23}H_{44}N_6O_4$ 468.638
Alkaloid from the venom of the spider *Agelenopsis aperta*.

N*,4-Dideoxy, 2,5-dihydroxy:* ***Agel 452a****. AG 452a. HO 452*
[133805-35-3]
$C_{23}H_{44}N_6O_3$ 452.639
Alkaloid from the venom of the spiders *Agelenopsis aperta* and *Hololena curta*.

$N^{17'}$*-De(aminopropyl),* $N^{17'}$*-(aminoiminomethyl),* N*-deoxy:* ***PB 421***
[333401-98-2]
$C_{21}H_{39}N_7O_2$ 421.585
Alkaloid from the venom of the spider *Paracoelotes birulai*.

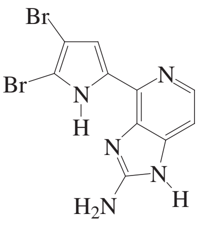
[128550-24-3]

Jasys, V.J. *et al., J.A.C.S.*, 1990, **112**, 6696-6704 (*isol, synth, ms, struct*)

Chesnov, S. *et al., Helv. Chim. Acta*, 2000, **83**, 3295-3305; 2001, **84**, 2178-2197 (*PB 421, Agel 452a*)

Ageladine A A-177

[643020-13-7]



$C_{10}H_7Br_2N_5$ 357.007

Isol. from *Agelas nakamurai*. Antiangiogenic matrixmetalloproteinase inhibitor. Yellow powder (as di-TFA salt). λ_{max} 227 (ϵ 15400); 250 (ϵ 9960); 381 (ϵ 12200) (MeOH) (di-TFA salt).

Fujita, M. *et al., J.A.C.S.*, 2003, **125**, 15700-15701 (*Ageladine A*)

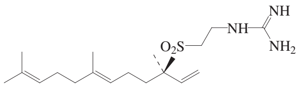
Shengule, S.R. *et al., Org. Lett.*, 2006, **8**, 4083-4084 (*synth*)

Meketa, M.L. *et al., J.O.C.*, 2007, **72**, 4892-4899 (*synth*)

Meketa, M.L. *et al., Tetrahedron*, 2007, **63**, 9112-9119 (*synth*)

Agelasidine A A-178

2-[[(1-Ethenyl-1,5,9-trimethyl-4,8-decadienyl)sulfonyl]ethyl]guanidine, 9CI



(*R*)*-form*

$C_{18}H_{33}N_3O_2S$ 355.544

(*R*)*-form* [915159-59-0]
Isol. from *Agelas clathrodes*. Oil. $[\alpha]_D^{20}$ -14.5 (c, 1.5 in MeOH).

(*S*)*-form*
Isol. from the Okinawan sea sponge *Agelas nakamurai* and from a Pacific sponge *Agelas* sp. Shows antispasmodic and antibacterial activity. Unstable yellow oil; cryst. + ⅓ H_2O (EtOAc)(as hydrochloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 108-108.5° (hydrochloride). $[\alpha]_D^{25}$ +19.1 (c, 1 in MeOH) (hydrochloride). λ_{max} 227 (ϵ 5400); 265 (ϵ 1800) (EtOH) (Berdy). λ_{max} 226 (ϵ 4000); 270 (ϵ 2000) (EtOH/HCl) (Berdy).

Capon, R.J. *et al., J.A.C.S.*, 1984, **106**, 1819-1822 (*isol, uv, ir, pmr, cmr, ms*)

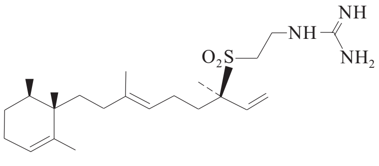
Nakamura, H. *et al., J.O.C.*, 1985, **50**, 2494-2497 (*isol, uv, ir, pmr, cmr*)

Ichikawa, Y. *et al., J.C.S. Perkin 1*, 1992, 1497-1500 (*synth*)

Medeiros, M.A. *et al., Z. Naturforsch., C*, 2006, **61**, 472-476 (*R-form, isol, pmr, cmr*)

Agelasidine B A-179

[96617-50-4]

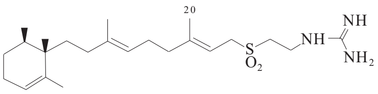


$C_{23}H_{41}N_3O_2S$ 423.662

Isol. from the Okinawan sea sponge *Agelas nakamurai*. Shows antispasmodic and antibacterial activity. Syrup (as hydrochloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ -2.5 (c, 0.43 in MeOH).

Nakamura, H. *et al., J.O.C.*, 1985, **50**, 2494 (*isol, uv, ir, pmr, cmr, struct*)

Agelasidine C A-180



(+)–*form*

$C_{23}H_{41}N_3O_2S$ 423.662

(+)*-form* [96617-52-6]
Isol. from the sponges *Agelas nakamurai* and *Agelas dispar*. Shows antispasmodic and antibacterial activity. Syrup (as hydrochloride). Sol. MeOH, $CHCl_3$. $[\alpha]_D^{25}$ +8.5 (c, 2.0 in MeOH) (hydrochloride).

(-)*-form* [139757-42-9]
Isol. from *Agelas clathrodes*. Oil. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{29}$ -5.6 (c, 7.2 in MeOH).

20-Hydroxy: ***Agelasidine D***
[139680-61-8]
$C_{23}H_{41}N_3O_3S$ 439.661
Isol. from *Agelas clathrodes*. Oil. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{29}$ -3.6 (c, 2.75 in MeOH).

[96617-52-6]

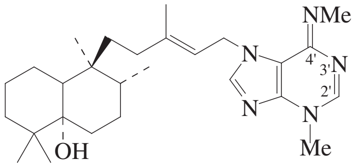
Nakamura, H. *et al., J.O.C.*, 1985, **50**, 2494-2498 (*isol, uv, ir, pmr, cmr, struct*)

Asao, K. *et al., Chem. Lett.*, 1989, 1813-1814 (*synth*)

Morales, J.J. *et al., J. Nat. Prod.*, 1992, **55**, 389-394 (*isol*)

Agelasimine A A-181

[114216-85-2]



$C_{27}H_{43}N_5O$ 453.67

Metab. from the marine sponge *Agelas mauritiana*. Exhibits cytotoxicity, inhibition of adenosine transfer into rabbit erythrocytes, $Ca^{2\oplus}$-channel antagonistic action and α_1 adrenergic blockade. Yellowish oil. Sol. MeOH, EtOH, $CHCl_3$. $[\alpha]_D^{25}$ +2.3 (MeOH). λ_{max} 223 (ϵ 9700); 287 (ϵ 14700) (MeOH) (Berdy).

*2′,3′-Dihydro, 3′*N*-Me,* $N^{4'}$*-de-Me:* ***Agelasimine B***
[114216-87-4]
$C_{27}H_{45}N_5O$ 455.685
Metab. from the marine sponge *Agelas mauritiana*. Exhibits cytotoxicity, inhibition of adenosine transfer into rabbit erythrocytes, $Ca^{2\oplus}$-channel antagonistic action and α_1 adrenergic blockade. Viscous yellowish oil. Sol. MeOH, $CHCl_3$, EtOH. $[\alpha]_D^{25}$ +2.46 (MeOH). λ_{max} 245 (ϵ 7100); 327 (ϵ 5400) (MeOH) (Berdy).

Fathi-Afshar, R. *et al., Can. J. Chem.*, 1988, **66**, 45 (*isol, uv, ir, pmr, cmr, ms, struct*)

Ohba, M. *et al., Tetrahedron*, 1997, **53**, 16977-16986 (*synth, abs config*)

Agelasine† A-182

Struct. unknown

$C_{26}H_{40}N_5^{\oplus}$ 422.635

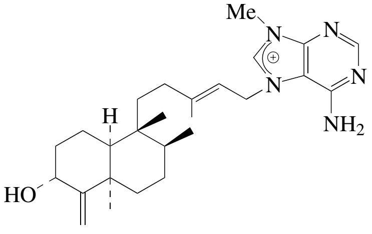
Quaternary 9-methyladenine deriv. of an unidentified bicyclic diterpene. Isol. from the sponge *Agelas dispar*. Cryst. (butanone/THF) (as chloride). Mp 197-200°

dec. (chloride). Mp of chloride does not appear to correspond with any of the Agelasines of known struct. λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

Cullen, E. *et al., Can. J. Chem.*, 1975, **53**, 1690-1691 (*isol, uv, ir, pmr, ms*)

Agelasine I A-183

[205382-10-1]



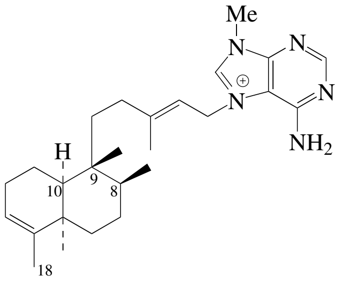
$C_{26}H_{40}N_5O^{\oplus}$ 438.635

Isol. from a sponge *Agelas* sp. Amorph. solid (as chloride). $[\alpha]_D$ -2.5 (c, 0.2 in MeOH). λ_{max} 272 (ϵ 8230) (MeOH).

Fu, X. *et al., J. Nat. Prod.*, 1998, **61**, 548-550 (*isol, uv, ir, pmr, cmr*)

Agelasine A† A-184

[56271-74-0]



$C_{26}H_{40}N_5^{\oplus}$ 422.635

Constit. of the Okinawan sponge *Agelas nakamurai*. ATPase inhibitor, spasmolytic agent, smooth muscle contractant. Cryst. (as chloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 173-174° (chloride). $[\alpha]_D^{25}$ -31.3 (c, 0.59 in MeOH). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

18-Hydroxy: ***Agelasine H***

[205382-09-8]

$C_{26}H_{40}N_5O^{\oplus}$ 438.635

Constit. of an *Agelas* sp. Amorph. solid (as chloride). $[\alpha]_D$ -63.9 (c, 0.36 in MeOH). λ_{max} 272 (ϵ 9015) (MeOH).

*18-Hydroxy, 18-*O*-(2-pyrrolecarbonyl):* ***Ageline B***

[88874-28-6]

[88855-18-9 , 88855-19-0]

$C_{31}H_{43}N_6O_2^{\oplus}$ 531.72

Constit. of sponge *Agelas* sp. Active against gram-positive bacteria. ATPase inhibitor. Smooth muscle contractor. Phytotoxin. Weak ichthyotoxin. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 210 (ϵ); 274 (ϵ) (EtOH) (Derep). λ_{max} 268 (ϵ 8320) (MeOH) (Berdy). λ_{max} 212 (ϵ 18100); 272 (ϵ 10111) (EtOH) (Berdy). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Berdy).

*18-Hydroxy, 18-*O*-(4-bromo-2-pyrrolecarbonyl):* ***Agelasine G***

[142808-37-5]

$C_{31}H_{42}BrN_6O_2^{\oplus}$ 610.616

Isol. from the Okinawan marine sponge *Agelas* sp. Exhibits cytotoxicity against murine lymphoma L1210 cells *in vitro*. $[\alpha]_D^{27}$ -85 (c, 0.02 in $CHCl_3$) (as chloride). λ_{max} 212 (ϵ 24000); 272 (ϵ 19000) (MeOH) (Berdy).

8,9,10-Triepimer: ***Agelasine B***

[92664-76-1]

$C_{26}H_{40}N_5^{\oplus}$ 422.635

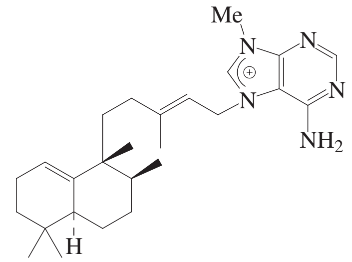
Constit. of *Agelas nakamurai*. ATPase inhibitor, spasmolyic agent. Cryst. (as chloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 167-170° (chloride). $[\alpha]_D^{25}$ -21.5 (c, 1.00 in MeOH). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

Cullen, E. *et al., Can. J. Chem.*, 1975, **53**, 1690-1691 (*isol*)
Capon, R.J. *et al., J.A.C.S.*, 1984, **106**, 1819-1822 (*Ageline B*)
Nakamura, H. *et al., Tet. Lett.*, 1984, **25**, 2989-2992 (*uv, pmr, cmr, struct*)
Hideo, I. *et al., Chem. Comm.*, 1985, 774-775 (*Ageline B, synth*)
Wu, H. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2495-2504 (*isol, pmr, cmr, uv, Agelasine B*)
Ishida, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 766-767 (*Agelasine G*)
Piers, E. *et al., J.C.S. Perkin 1*, 1995, 963-966 (*synth*)
Fu, X. *et al., J. Nat. Prod.*, 1998, **61**, 548-550 (*Agelasine H*)

Agelasine C A-185

[92664-78-3]

[92664-79-4 (chloride)]



$C_{26}H_{40}N_5^{\oplus}$ 422.635

Stereochem. revised in 2005. Isol. from the sponge *Agelas nakamurai*. Shows antimicrobial activity. ATP-ase inhibitor. Spasmolytic agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 176-179° (as chloride). $[\alpha]_D^{25}$ -55.1 (c, 2.04 in MeOH) (chloride). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

5,9-Diepimer: ***Epiagelasine C***

[187825-31-6]

$C_{26}H_{40}N_5^{\oplus}$ 422.636

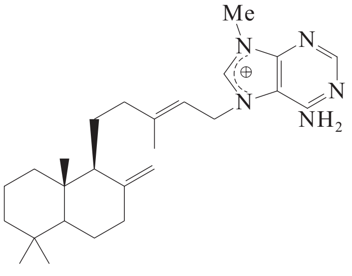
Constit. of sponge *Agelas mauritiana*. Antifouling substance against macroalgae. Powder (as chloride). $[\alpha]_D^{25}$ +33.9 (c, 0.056 in MeOH) (chloride). Stereochem. revised in 2005. λ_{max} 273 (ϵ 8140) (MeOH).

Nakamura, H. *et al., Tet. Lett.*, 1984, **25**, 2989-2992 (*isol, uv, pmr, cmr*)
Wu, H. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2495-2504 (*isol, pmr, cmr, uv*)
Hattori, T. *et al., J. Nat. Prod.*, 1997, **60**, 411-413 (*5-epimer*)
Marcos, I. *et al., Tetrahedron*, 2005, **61**, 11672-11678 (*synth, abs config*)

Agelasine D A-186

[92664-80-7]

[92664-81-8 (chloride)]



$C_{26}H_{40}N_5^{\oplus}$ 422.635

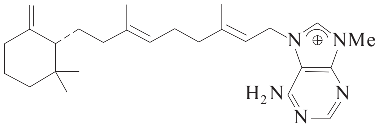
Isol. from the Okinawan sea sponge *Agelas nakamurai*. Shows antimicrobial activity. Spasmolytic agent. Na/K ATP-ase inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 175-176° (as chloride). $[\alpha]_D^{25}$ +10.4 (c, 1.1 in MeOH) (chloride). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

Nakamura, H. *et al., Tet. Lett.*, 1984, **25**, 2989-2992 (*uv, pmr, cmr, struct*)
Wu, H. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2495-2504 (*isol, uv, pmr, cmr*)
Utenova, B.T. *et al., Tet. Lett.*, 2004, **45**, 4233-4235 (*synth*)
Vik, A. *et al., J. Nat. Prod.*, 2006, **69**, 381-386 (*synth, activity*)

Agelasine E A-187

[92599-00-3]

[92599-01-4 (chloride)]



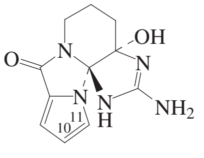
$C_{26}H_{40}N_5^{\oplus}$ 422.635

Isol. from the Okinawan sea sponge *Agelas nakamurai*. ATP-ase inhibitor, spasmolytic agent, shows antimicrobial props. Powder (as chloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 180-182° (chloride). $[\alpha]_D^{23}$ -17.1 (c, 1.88 in MeOH) (chloride). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

Wu, H. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2495-2504 (*uv, pmr, cmr, ms, struct*)
Bakkestuen, A.K. *et al., Org. Biomol. Chem.*, 2005, **3**, 1025-1033 (*synth*)

Agelaspongin A-188

[122893-39-4]



Relative Configuration

$C_{11}H_{13}N_5O_2$ 247.256

CA numbering shown. Synthetic. Cryst. (MeOH). Mp 220° dec.

Hydrochloride:
Cryst. (EtOH). Mp 250° dec.

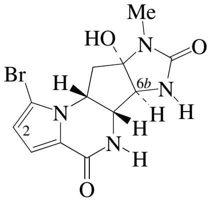
10,11-Dibromo: ***Dibromoagelaspongin***
[122893-38-3]
$C_{11}H_{11}Br_2N_5O_2$ 405.048
Isol. from an *Agelas* sp. Glucanase inhibitor. Yellow-green cryst. (MeOH/ Me_2CO) (as hydrochloride). Mp 233-235° dec. (hydrochloride). λ_{max} 235 (ϵ 11250); 290 (ϵ 7420) (MeOH) (Berdy).

10,11-Dibromo, Me ether: ***Dibromoagelaspongin methyl ether***
[934842-17-8]
$C_{12}H_{13}Br_2N_5O_2$ 419.075
Isol. from *Agelas dispar.*

Fedoreyev, S.A. *et al., Tetrahedron*, 1989, **45**, 3487-3492 (*isol, pmr, cmr, ms, cryst struct*)
Pina, I.C. *et al., J. Nat. Prod.*, 2007, **70**, 613-617 (*dibromo Me ether*)
Feldman, K.S. *et al., J.A.C.S.*, 2008, **130**, 14964-14965 (*dibromo, synth*)

Agelastatin A A-189

[152406-28-5]



Absolute Configuration

$C_{12}H_{13}BrN_4O_3$ 341.164

Alkaloid from the sponge *Agelas dendromorpha* and *Cymbastela* sp. Exhibits marked cytotoxicity; insecticide. Antineoplastic agent. Prevents metastatic cancer spread. $[\alpha]_D^{20}$ -84.3 (c, 0.3 in EtOH) (as *N,N,O*-tri-Me). Not obt. completely pure. λ_{max} 203 (ϵ 12400); 232 (ϵ 8400); 279 (ϵ 11900) (EtOH) (Derep).

N-*De-Me:* ***Agelastatin D***
[201338-45-6]
$C_{11}H_{11}BrN_4O_3$ 327.137
Alkaloid from the sponge *Cymbastela* sp. Insecticide. Solid. λ_{max} 227 (ϵ 7900); 277 (ϵ 10800) (MeOH).

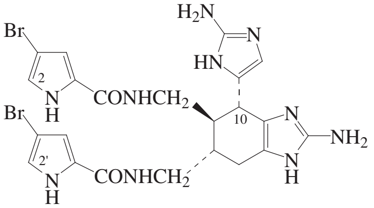
2-Bromo: ***Agelastatin B***
[159903-65-8]
$C_{12}H_{12}Br_2N_4O_3$ 420.06
Minor alkaloid from *Agelas dendromorpha.* $[\alpha]_D$ -84.4 (c, 0.49 in EtOH) (as *N,N,O*-tri-Me). Obt. as insep. mixt. with Agelastatin A but characterised as the tri-Me deriv.

6b-Hydroxy: ***Agelastatin C***
[201338-44-5]
$C_{12}H_{13}BrN_4O_4$ 357.163
Alkaloid from the sponge *Cymbastela* sp. Cytotoxic; insecticide. Solid. $[\alpha]_D$ -5 (c, 0.06 in MeOH). λ_{max} 228 (ϵ 7900); 278 (ϵ 11000) (MeOH).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1994, **77**, 1895; 1996, **79**, 727 (*Agelastatins A,B*)
Hong, T.W. *et al., J. Nat. Prod.*, 1998, **61**, 158-161 (*Agelastatins C,D*)
Stien, D. *et al., J.A.C.S.*, 1999, **121**, 9574-9579 (*synth*)
Feldman, K.S. *et al., J.O.C.*, 2002, **67**, 7096-7109 (*synth*)
Hale, K.J. *et al., Org. Lett.*, 2003, **5**, 2927-2930 (*synth*)
Domostoj, M.M. *et al., Org. Lett.*, 2004, **6**, 2615-2618 (*synth*)
Davis, F.A. *et al., Org. Lett.*, 2005, **7**, 621-623 (*synth*)
Trost, B.M. *et al., J.A.C.S.*, 2006, **128**, 6054-6055 (*synth*)
Ichikawa, Y. *et al., Org. Lett.*, 2007, **9**, 2989-2992 (*synth*)
Mason, C.K. *et al., Mol. Cancer Ther.*, 2008, **7**, 548-558 (*agelastatin A, pharmacol*)

Ageliferin A-190

[117417-64-8]



$C_{22}H_{24}Br_2N_{10}O_2$ 620.305

Alkaloid from the marine sponges *Agelas conifera*, *Agelas novaecaledoniae*, *Agelas* cf. *mauritiana* and *Xestospongia* sp. Potent actomyosin ATPase activator. Antifouling agent. Somatostatin antagonist. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{33}$ +15.5 (c, 0.11 in MeOH). λ_{max} 204 (ϵ 25500); 220 (ϵ 27100); 267 (ϵ 25900); 393 (ϵ 300) (MeOH) (Derep).

*1'-*N*-Me:* **1'-N-*Methylageliferin***
[175861-97-9]
$C_{23}H_{26}Br_2N_{10}O_2$ 634.332
Alkaloid from the sponge *Astrosclera willeyana*. Pale yellow glass (as bis(trifluoroacetate)). $[\alpha]_D$ +40 (c, 0.01 in MeOH).

*1,1'-Di-*N*-Me:* **N^{1},N$^{1'}$-*Dimethylageliferin***
[175861-98-0]
$C_{24}H_{28}Br_2N_{10}O_2$ 648.359
Alkaloid from the sponge *Astrosclera willeyana*. Pale buff glass (as dihydrochloride). $[\alpha]_D$ +40 (c, 0.01 in MeOH).

2-Bromo: ***2-Bromoageliferin***
[117417-67-1]
$C_{22}H_{23}Br_3N_{10}O_2$ 699.201
Alkaloid from the sponges *Agelas conifera*, *Agelas* cf. *mauritiana* and *Astrosclera willeyana*. Potent actomyosin ATPase activator. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{33}$ +8.8 (c, 0.08 in MeOH). λ_{max} 203 (ϵ 30600); 220 (ϵ 26300); 270 (ϵ 24500); 396 (ϵ 700) (MeOH) (Derep). λ_{max} 204 (ϵ 15000); 222 (ϵ 12200); 274 (ϵ 12500); 396 (ϵ 700) (EtOH) (Berdy).

*2-Bromo, 1'-*N*-Me:* **1'-N-*Methyl-2-bromoageliferin***
[175862-01-8]
$C_{23}H_{25}Br_3N_{10}O_2$ 713.228
Alkaloid from the sponge *Astrosclera willeyana*. Off-white glass (as bis(trifluoroacetate)). $[\alpha]_D$ +50 (c, 0.01 in MeOH).

*2'-Bromo, 1'-*N*-Me:* **1'-N-*Methyl-2'-bromoageliferin***
[175862-02-9]
$C_{23}H_{25}Br_3N_{10}O_2$ 713.228
Alkaloid from the sponge *Astrosclera willeyana*. Off-white glass (as bis(trifluoroacetate)). $[\alpha]_D$ +40 (c, 0.01 in MeOH).

2,2'-Dibromo: ***2,2'-Dibromoageliferin***
[117417-69-3]
$C_{22}H_{22}Br_4N_{10}O_2$ 778.098
Alkaloid from the sponges *Agelas conifera*, *Agelas* cf. *mauritiana* and *Astrosclera willeyana*. Potent actomyosin ATPase activator. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{33}$ +3 (c, 0.1 in MeOH). λ_{max} 204 (ϵ 12200); 220 (ϵ 9100); 278 (ϵ 8200); 394 (ϵ 300) (no solvent reported) (Derep). λ_{max} 202 (ϵ 24300); 214 (ϵ 24500); 274 (ϵ 25000) (MeOH) (Derep). λ_{max} 204 (ϵ 12200); 220 (ϵ 9100); 278 (ϵ 8200); 394 (ϵ 300) (EtOH) (Berdy).

*2,2'-Dibromo, 1'-*N*-Me:* **1'-N-*Methyl-2,2'-dibromoageliferin***
[175862-03-0]
$C_{23}H_{24}Br_4N_{10}O_2$ 792.124
Alkaloid from the sponge *Astrosclera willeyana*. Off-white glass (as bis(trifluoroacetate)). $[\alpha]_D$ +30 (c, 0.01 in MeOH).

*3'-Debromo, 2'-bromo, 1'-*N*-Me:* **1'-N-*Methylisoageliferin***
[175861-99-1]
$C_{23}H_{26}Br_2N_{10}O_2$ 634.332
Alkaloid from the sponge *Astrosclera willeyana*. Pale yellow glass (as bis(trifluoroacetate)). $[\alpha]_D$ +40 (c, 0.01 in MeOH).

*3'-Debromo, 2'-bromo, 1,1'-di-*N*-Me:* **N^{1},N$^{1'}$-*Dimethylisoageliferin***
[175862-00-7]
$C_{24}H_{28}Br_2N_{10}O_2$ 648.359
Alkaloid from the sponge *Astrosclera willeyana*. Off-white glass (as dihydrochloride). $[\alpha]_D$ +40 (c, 0.01 in MeOH).

10-Epimer: ***Nagelamide E***
[690627-58-8]
$C_{22}H_{24}Br_2N_{10}O_2$ 620.305
Alkaloid from an *Agelas* sp. Amorph. solid. $[\alpha]_D^{17}$ -11.3 (c, 1 in MeOH). λ_{max} 202 (ϵ 32000); 215 (sh) (ϵ 18000); 272 (ϵ 17200) (MeOH).

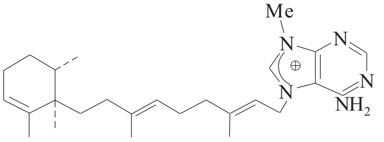
10-Epimer, 2-bromo: ***Nagelamide F***
[690627-59-9]
$C_{22}H_{23}Br_3N_{10}O_2$ 699.202
Alkaloid from an *Agelas* sp. Amorph. solid. $[\alpha]_D^{17}$ -14.1 (c, 1 in $CHCl_3$). λ_{max} 202 (ϵ 24000); 216 (sh) (ϵ 20100); 272 (ϵ 17700) (MeOH).

10-Epimer, 2,2′-dibromo: ***Nagelamide G***
[690627-60-2]
$C_{22}H_{22}Br_4N_{10}O_2$ 778.098
Alkaloid from an *Agelas* sp. Inhibitor of protein phosphatase 2A. Amorph. solid. $[\alpha]_D^{17}$ +6.7 (c, 1 in MeOH). λ_{max} 202 (ϵ 32000); 215 (sh) (ϵ 28900); 277 (ϵ 27400) (MeOH).

Kobayashi, J. *et al., Tetrahedron*, 1990, **46**, 5579-5586 (*isol, pmr, cmr, struct*)
Keifer, P.A. *et al., J.O.C.*, 1991, **56**, 2965-2975; 6728 (*isol*)
Vassas, A. *et al., Planta Med.*, 1996, **62**, 28-30 (*isol, activity*)
Williams, D.H. *et al., Tetrahedron*, 1996, **52**, 5381-5390 (*N-Methylageliferins*)
Kawasaki, I. *et al., Tet. Lett.*, 2002, **43**, 4377-4380 (*deriv, synth*)
Hoffmann, H. *et al., Synthesis*, 2003, 1753-1783 (*rev*)
Endo, T. *et al., J. Nat. Prod.*, 2004, **67**, 1262-1267 (*Nagelamides*)
O'Malley, D.P. *et al., J.A.C.S.*, 2007, **129**, 4762-4775; 7702 (*synth*)

Ageline A **A-191**

Agelasine F
[88929-28-6]
[8885-51-6]

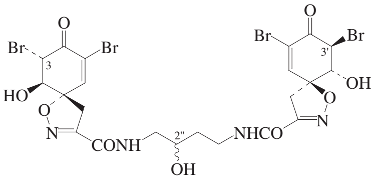


$C_{26}H_{40}N_5^{\oplus}$ 422.635
Constit. of sponge *Agelas* sp. Active against gram-positive bacteria and fungi. ATPase inhibitor, weak ichthyotoxin. Active against *Mycobacterium tuberculosis*. Plates (MeCN) or powder (as chloride). Mp 178-180° (chloride). $[\alpha]_D^{25}$ -5.5 (c, 2.5 in MeOH). $[\alpha]_D$ -8.4 (c, 3 in $CHCl_3$). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

Capon, R.J. *et al., J.A.C.S.*, 1984, **106**, 1819-1822 (*isol, uv, pmr, cmr*)
Wu, H. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2495-2504 (*isol, pmr, cmr, uv, struct*)
Mangalindan, G.C. *et al., Planta Med.*, 2000, **66**, 364-365 (*activity*)

Agelocaissarine A₁ **A-192**

[927409-64-1]



$C_{22}H_{22}Br_4N_4O_9$ 806.053
Related to Aerothionin, A-158. Constit. of *Aplysina caissara*. Obt. as an inseparable mixt. with Agelocaissarine A_2.

3,3′-Diepimer: ***Agelocaissarine A₂***
[927409-65-2]
$C_{22}H_{22}Br_4N_4O_9$ 806.053
Constit. of *Aplysina caissara*.

Homologue: ***Agelocaissarine B₁***
[927409-66-3]
$C_{23}H_{24}Br_4N_4O_9$ 820.08
Constit. of *Aplysina caissara*. Has a C_5 bridging chain (-$CH_2CH(OH)CH_2CH_2CH_2$-) instead of C_4. Obt. as an inseparable mixt. with Agelocaissarine B_2.

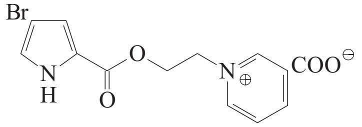
Homologue, 2′′-deoxy: ***Aplysinone B***
[943837-23-8]
$C_{23}H_{24}Br_4N_4O_8$ 804.081
Constit. of *Aplysina gerardogreeni*. Amorph. solid. $[\alpha]_D^{25}$ -4 (c, 0.1 in Me_2CO). Has a C_5 bridging chain instead of C_4.

Homologue, 3,3′-diepimer: ***Agelocaissarine B₂***
[927409-67-4]
$C_{23}H_{24}Br_4N_4O_9$ 820.08
Constit. of *Aplysina caissara*. Has a C_5 bridging chain (-$CH_2CH(OH)CH_2CH_2CH_2$-) instead of C_4.

De Lira, T.O. *et al., J. Braz. Chem. Soc.*, 2006, **17**, 1233-1240 (*Agelocaissarines A_1,A_2,B_1,B_2*)
Hernández-Guerrero, C.J. *et al., Bioorg. Med. Chem.*, 2007, **15**, 5275-5282 (*Aplysinone B*)

Agelongine **A-193**

[163564-84-9]



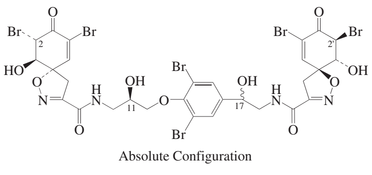
$C_{13}H_{11}BrN_2O_4$ 339.145
Alkaloid from *Agelas longissima* and *Axinella damicornis*. Exhibits antiserotonergic activity. Amorph. solid. Sol. MeOH, butanol. λ_{max} 262 (log ϵ 4.2) (MeOH).

Debromo: ***Daminine***
[862288-76-4]
$C_{13}H_{12}N_2O_4$ 260.249
Alkaloid from *Axinella damicornis*. Amorph. solid. Mp 193° dec.

Cafieri, F. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 799-804 (*isol, uv, pmr, cmr*)
Aiello, A. *et al., Tetrahedron*, 2005, **61**, 7266-7270 (*Daminine*)

Agelorin A **A-194**

[149998-47-0]



Absolute Configuration

$C_{29}H_{26}Br_6N_4O_{11}$ 1085.969
Hydrol. prod. of Fistularin 3, F-70 on standing. Metab. from the tropical marine sponge *Agelas oroides*. Shows antibacterial activity. Amorph. off-white powder. $[\alpha]_D^{25}$ -17.1 (c, 1.26 in Me_2CO). λ_{max} 220 (ϵ 12600); 250 (ϵ 7740) (EtOH) (Berdy).

11,17-Dideoxy: ***11,17-Dideoxyagelorin A***
$C_{29}H_{26}Br_6N_4O_9$ 1053.97
Isol. from the sponge *Suberea* aff. *praetensa*.

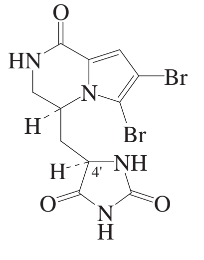
2,2′-Diepimer: ***Agelorin B***
[150133-30-5]
$C_{29}H_{26}Br_6N_4O_{11}$ 1085.969
Isol. from *Agelas oroides*. Shows antibacterial activity. Amorph. powder. $[\alpha]_D^{25}$ +50 (c, 0.27 in Me_2CO). λ_{max} 215 (ϵ 12570); 250 (ϵ 7940) (EtOH) (Berdy).

2,2′-Diepimer, 11,17-dideoxy: ***11,17-Dideoxyagelorin B***
$C_{29}H_{26}Br_6N_4O_9$ 1053.97
Isol. from the sponge *Suberea* aff. *praetensa*.

König, G.M. *et al., Heterocycles*, 1993, **36**, 1351 (*isol, uv, ir, pmr, cmr, ms*)
Kijjoa, A. *et al., Z. Naturforsch., C*, 2001, **56**, 1116-1119 (*11,17-Dideoxyagelorins*)
Rogers, E.W. *et al., J. Nat. Prod.*, 2005, **68**, 891-896 (*stereochem*)
Bardhan, S. *et al., Org. Lett.*, 2006, **8**, 927-930 (*stereochem*)

Agesamide A **A-195**

[911296-34-9]



Relative Configuration

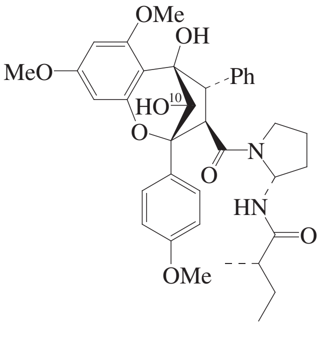
$C_{11}H_{10}Br_2N_4O_3$ 406.033
Related to Cyclooroidin, C-887. Isol. from an *Agelas* sp. Amorph. solid. $[\alpha]_D^{20}$ +3.2 (c, 0.5 in MeOH). λ_{max} 204 (ϵ 12000); 282 (ϵ 2800) (MeOH).

4′-Epimer: ***Agesamide B***
[911296-35-0]
$C_{11}H_{10}Br_2N_4O_3$ 406.033
Isol. from an *Agelas* sp. Amorph. solid. $[\alpha]_D^{20}$ +2.8 (c, 0.5 in MeOH). λ_{max} 204 (ϵ 12300); 282 (ϵ 3050) (MeOH).

Tsuda, M. *et al., Org. Lett.*, 2006, **8**, 4235-4238 (*isol, pmr, cmr*)
Trost, B.M. *et al., Org. Lett.*, 2007, **9**, 2357-2359 (*synth*)

Aglaforbesine A **A-196**

[177262-33-8]



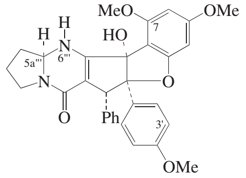
$C_{36}H_{42}N_2O_8$ 630.736
Alkaloid from *Aglaia forbesii*. Amorph. solid. $[\alpha]_D^{20}$ -18 (c, 1 in MeOH). λ_{max} 271 (log ε 3.25) (MeOH).

10-Epimer: ***Aglaforbesine B***
[177468-86-9]
$C_{36}H_{42}N_2O_8$ 630.736
Alkaloid from *Aglaia forbesii*. Amorph. solid. $[\alpha]_D^{20}$ +1 (c, 1 in MeOH). λ_{max} 270 (log ε 3.25) (MeOH).

Dumontet, V. *et al., Tetrahedron*, 1996, **52**, 6931-6942 (*isol, uv, ir, pmr, cmr*)

Aglaiastatin **A-197**

Aglaroxin D
[176785-78-7]



Absolute Configuration

$C_{31}H_{30}N_2O_6$ 526.588
Isol. from leaves of *Aglaia odorata* and *Aglaia roxburghiana*. Protein synthesis inhibitor. K-Ras transformed fibroblast morphology inducer. Powder + 1½H_2O. Mp 157-160°. $[\alpha]_D^{23}$ +59.7 (c, 0.3 in MeOH). λ_{max} 281 (ε 4163); 304 (ε 4480) (MeOH).

5a''',N$^{6'''}$-Didehydro: ***Dehydroaglaiastatin***. *Didehydroaglaiastatin*
[155595-93-0]
$C_{31}H_{28}N_2O_6$ 524.572
Isol. from roots of *Aglaia odorata* and twigs of *Aglaia duppereana* (Meliaceae). Protein synthesis inhibitor. Plates (CH_2Cl_2/MeOH). Mp 256-257°. $[\alpha]_D^{20}$ -50.1 (c, 0.41 in $CHCl_3$). λ_{max} 215 (ε 50000); 234 (ε 19000); 272 (ε 6000) (EtOH) (Derep).

*5a''',N$^{6'''}$-Didehydro, 7-*O*-de-Me:* ***Marikarin***
[349642-85-9]
$C_{30}H_{26}N_2O_6$ 510.545
Alkaloid from *Aglaia gracilis*. Oil. $[\alpha]_D^{20}$ -45 (c, 0.3 in $CHCl_3$). λ_{max} 273 (MeOH).

3'-Hydroxy, 5a''',N$^{6'''}$-didehydro: ***Didehydro-3'-hydroxyaglaiastatin***
[259143-58-3]
$C_{31}H_{28}N_2O_7$ 540.571
Isol. from *Aglaia duperreana*.

*3'-Hydroxy, 5a''',N$^{6'''}$-didehydro, 7-*O*-de-Me:* ***3'-Hydroxymarikarin***
[349484-01-1]
$C_{30}H_{26}N_2O_7$ 526.545
Alkaloid from *Aglaia gracilis*. Oil. $[\alpha]_D^{20}$ -53 (c, 0.1 in $CHCl_3$). λ_{max} 279 (MeOH).

3'-Methoxy, 5a''',N$^{6'''}$-didehydro: ***Aglaiformosanin***. *Didehydro-3'-methoxyaglaiastatin*
[371163-97-2]
$C_{32}H_{30}N_2O_7$ 554.598
Isol. from *Aglaia formosana*. Cytotoxic. Powder. Mp 260-262°. $[\alpha]_D^{22}$ -78.9 (c, 0.01 in $CHCl_3$). λ_{max} 213 (log ε 4.39); 256 (log ε 3.78); 274 (log ε 3.68) (MeOH).

Stereoisomer: [189343-27-9]
$C_{31}H_{30}N_2O_6$ 526.588
Isol. from twigs of *Aglaia duppereana*. $[\alpha]_D^{20}$ +45.7 (c, 0.19 in $CHCl_3$).

Kokpol, U. *et al., Chem. Comm.*, 1994, 773-774 (*isol, ir, pmr, cmr, cryst struct*)
Ohse, T. *et al., J. Nat. Prod.*, 1996, **59**, 650-652 (*isol, uv, ir, pmr, cmr, cryst struct*)
Pat. Coop. Treaty (WIPO), 1996, 96 04 284; *CA*, **124**, 335673h (*Aglaroxin D*)
Nugroho, B.W. *et al., Phytochemistry*, 1997, **44**, 1455-1461 (*isol, pmr, cmr, cd, ms*)
Watanabe, T. *et al., Chem. Comm.*, 1998, 1097-1098 (*synth*)
Chaidir, *et al., Phytochemistry*, 1999, **52**, 837-842 (*Didehydro-3'-hydroxyaglaiastatin*)
Watanabe, T. *et al., Heterocycles*, 2000, **53**, 1051-1064 (*synth*)
Greger, H. *et al., Phytochemistry*, 2001, **57**, 57-64 (*Marikarin, 3'-Hydroxymarikarin*)
Wang, S.-K. *et al., Planta Med.*, 2001, **67**, 555-557 (*Aglaiformosanin*)

Aglaidithioduline **A-198**

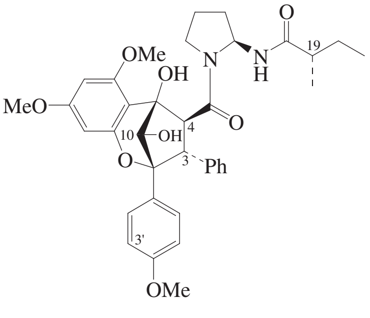
N,N'-Bis[3-(methylthio)-2-propenoyl]putrescine. Hemileptagline
MeSCH═CH
CONH$(CH_2)_4$NHCOCH═CHSMe
$C_{12}H_{20}N_2O_2S$ 256.368
Struct. of Hemileptagline revised in 2002.

(E,E)-form [261158-70-7]
Alkaloid from *Aglaia leptantha* and *Aglaia edulis*. Pale orange needles (MeOH). Mp 164-165°. λ_{max} 271 (log ε 4.6) (MeOH).

Saifah, E. *et al., Phytochemistry*, 1999, **52**, 1085-1088 (*Aglaidithioduline*)
Greger, H. *et al., J. Nat. Prod.*, 2000, **63**, 616-620 (*Hemileptagline*)
Detterback, R. *et al., Tetrahedron*, 2002, **58**, 6887-6893 (*synth*)

Aglaine B **A-199**

Aglaroxin K
[177262-32-7]
[251982-74-8 (Aglaroxin K)]



$C_{36}H_{42}N_2O_8$ 630.736
Alkaloid from *Aglaia argentea* and *Aglaia roxburghiana*. Amorph. powder. $[\alpha]_D^{20}$ -10 (c, 1 in MeOH). λ_{max} 272 (log ε 3.41) (MeOH).

5-Ac: *5-Acetylaglaine B*. ***Aglaroxin J***
[251982-73-7]
$C_{38}H_{44}N_2O_9$ 672.774
Alkaloid from the stem bark of *Aglaia roxburghiana*.

10-Ac: ***10-Acetylaglaine B***
[177468-88-1]
$C_{38}H_{44}N_2O_9$ 672.774
Alkaloid from the leaves of *Aglaia elliptica*. Amorph. powder. $[\alpha]_D^{20}$ +20.4 (c, 0.83 in MeOH).

3'-Hydroxy: ***3'-Hydroxyaglaine B***
[243136-41-6]
$C_{36}H_{42}N_2O_9$ 646.736
Alkaloid from *Aglaia odorata*. $[\alpha]_D^{20}$ -11.4 (c, 0.25 in $CHCl_3$).

10-Epimer: ***Deacetylaglaine A***
$C_{36}H_{42}N_2O_8$ 630.736
Alkaloid from *Aglaia gracilis*. Oil. $[\alpha]_D^{20}$ -14 (c, 0.1 in $CHCl_3$). Possible artifact. C-19 config. not determined. λ_{max} 271 ; 277 (sh) (MeOH).

10-Epimer, 10-Ac: ***Aglaine A***
[177262-31-6]
$C_{38}H_{44}N_2O_9$ 672.774
Alkaloid from *Aglaia argentea* and *Aglaia forbesii*. Amorph. powder. $[\alpha]_D^{20}$ -8 (c, 1 in MeOH). λ_{max} 272 (log ε 3.6) (MeOH).

*10-Epimer, 19,20-didehydro(*E*-):* ***Elliptifoline***
[319917-12-9]
$C_{36}H_{40}N_2O_8$ 628.721
Alkaloid from *Aglaia elliptifolia*. Cytotoxic agent. Powder. Mp 184-185°. $[\alpha]_D^{22}$ -88.9 (c, 0.6 in $CHCl_3$). λ_{max} 273 (log ε 3.36) (MeOH).

3,4-Diepimer: ***Aglaine C***
[177468-85-8]
$C_{36}H_{42}N_2O_8$ 630.736
Alkaloid from *Aglaia argentea*. Cryst. (MeOH). Mp 180°. $[\alpha]_D^{20}$ -105 (c, 1 in $CHCl_3$). λ_{max} 271 (log ε 3.27) (MeOH).

3,4-Diepimer, 3'-hydroxy: ***3'-Hydroxyaglaine C***
[243136-38-1]
$C_{36}H_{42}N_2O_9$ 646.736
Alkaloid from *Aglaia odorata*. $[\alpha]_D^{20}$ -103.4 (c, 0.43 in $CHCl_3$).

3,4-Diepimer, 19ξ-hydroxy: ***Aglaroxin L***
[251982-75-9]
$C_{36}H_{42}N_2O_9$ 646.736
Alkaloid from the stem bark of *Aglaia roxburghiana*. C-19 config. not determined.

3,4-Diepimer, 3',19-dihydroxy: ***3',19-Dihydroxyaglaine C***
[243136-39-2]
$C_{36}H_{42}N_2O_{10}$ 662.735
Alkaloid from *Aglaia odorata*. $[\alpha]_D^{20}$ -86 (c, 0.18 in $CHCl_3$). C-19 config. not determined.

3,4-Diepimer, 3'-methoxy, 19-hydroxy: ***19-Hydroxy-3'-methoxyaglaine C***
[243136-40-5]
$C_{37}H_{44}N_2O_{10}$ 676.762
Alkaloid from *Aglaia odorata*. $[\alpha]_D^{20}$ -111 (c, 0.18 in $CHCl_3$). C-19 config. not determined.

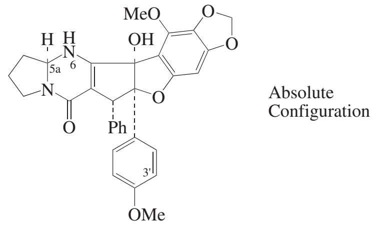
4,10-Diepimer, 10-Ac: ***4-Epiaglaine A***
[372119-00-1]
$C_{38}H_{44}N_2O_9$ 672.774

Alkaloid from the leaves of *Aglaia elliptica*. Amorph. powder. $[\alpha]_D^{20}$ -1 (c, 1 in $CHCl_3$).

Dumontet, V. *et al., Tetrahedron*, 1996, **52**, 6931-6942 (*isol, uv, ir, pmr, cmr*)
Molleyres, L.-P. *et al., Pestic. Sci.*, 1999, **55**, 486-503 (*Aglaroxins J,K,L*)
Nugroho, B.W. *et al., Phytochemistry*, 1999, **51**, 367-376 (*isol, derivs*)
Inada, A. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1226-1228 (*4-Epiaglaine A, 10-Acetylaglaine B*)
Wang, S.-K. *et al., J. Nat. Prod.*, 2001, **64**, 92-94 (*Elliptifoline*)
Greger, H. *et al., Phytochemistry*, 2001, **57**, 57-64 (*Deacetylaglaine A*)

Aglaroxin I **A-200**

[251982-72-6]



$C_{31}H_{28}N_2O_7$ 540.571
Alkaloid from the stem bark of *Aglaia roxburghiana*.

5a,6-Didehydro: ***Aglaroxin C***
[176785-77-6]
$C_{31}H_{26}N_2O_7$ 538.556
Alkaloid from *Aglaia roxburghiana*. Insecticide. λ_{max} 274 (ϵ 9600) (MeCN).

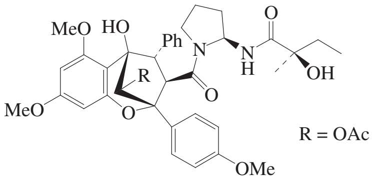
3′-Methoxy: ***Aglaroxin H***
[251982-71-5]
$C_{32}H_{30}N_2O_8$ 570.598
Alkaloid from the stem bark of *Aglaia roxburghiana*.

3′-Methoxy, 5a′′′,6-didehydro: ***Aglaroxin G***
$C_{32}H_{28}N_2O_8$ 568.582
Alkaloid from *Aglaia roxburghiana*.

Pat. Coop. Treaty (WIPO), 1996, 96 04 284; *CA*, **124**, 335673h (*Aglaroxin C*)
Molleyres, L.-P. *et al., Pestic. Sci.*, 1999, **55**, 494-497 (*Aglaroxins G-I*)

Aglaxiflorin C **A-201**

[269739-77-7]

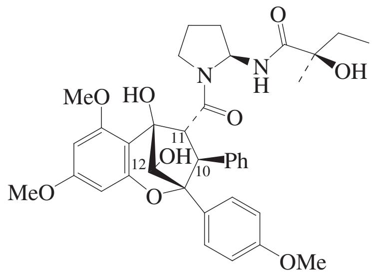


$C_{38}H_{44}N_2O_{10}$ 688.773
Flavagline compd. Alkaloid from *Aglaia laxiflora*. Cryst. ($CHCl_3$). Mp 147-149°. $[\alpha]_D^{25}$ +34.9 (c, 0.05 in $CHCl_3$). λ_{max} 222 (log ϵ 4.42); 272 (log ϵ 3.29) (MeOH).

Xu, Y.-J. *et al., J. Nat. Prod.*, 2000, **63**, 473-476

Aglaxiflorin D **A-202**

[269739-78-8]



$C_{36}H_{42}N_2O_9$ 646.736
Flavagline compd. Alkaloid from *Aglaia laxiflora*. Cryst. ($CHCl_3$). Mp 131-133°. $[\alpha]_D^{25}$ -102.1 (c, 0.04 in $CHCl_3$). λ_{max} 210 (log ϵ 5.62); 214 (log ϵ 5.66); 268 (log ϵ 4.66) (MeOH).

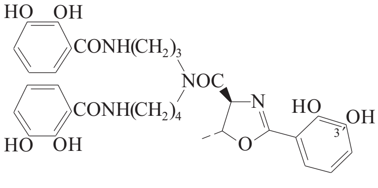
12-Epimer, 12-Ac: ***Aglaxiflorin B***
[269739-75-5]
$C_{38}H_{44}N_2O_{10}$ 688.773
Alkaloid from *Aglaia laxiflora*. Cryst. ($CHCl_3$). Mp 158-160°. $[\alpha]_D^{25}$ -105.5 (c, 0.13 in $CHCl_3$). λ_{max} 222 (log ϵ 4.47); 274 (log ϵ 3.66) (MeOH).

10,12-Diepimer, 12-Ac: ***Aglaxiflorin A***
[269739-76-6]
$C_{38}H_{44}N_2O_{10}$ 688.773
Alkaloid from *Aglaia laxiflora*. Cryst. ($CHCl_3$). Mp 217-219°. $[\alpha]_D^{25}$ +8.1 (c, 0.12 in $CHCl_3$). λ_{max} 214 (log ϵ 4.64); 268 (log ϵ 3.73) (MeOH).

Xu, Y.-J. *et al., J. Nat. Prod.*, 2000, **63**, 473-476

Agrobactin **A-203**

[70393-50-9]



$C_{32}H_{36}N_4O_{10}$ 636.657
Isol. from *Agrobacterium tumefaciens*. Siderophore. Cryst. (EtOAc/hexane). Sol. H_2O; fairly sol. MeOH. Dec. at 108-112°. λ_{max} 252 ; 316 (H_2O) (Berdy).

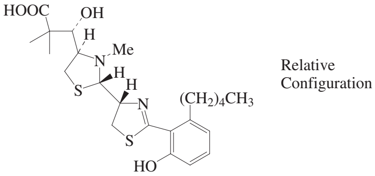
3′-Deoxy: ***Parabactin***. *Parabactin A*
[74149-70-5]
$C_{32}H_{36}N_4O_9$ 620.658
From *Paracoccus denitrificans*. Siderophore with antitumour and antiviral activity. Iron chelator. Cryst. (EtOAc/hexane). Sol. MeOH, Et_2O, bases; poorly sol. H_2O. Mp 114-117°. $[\alpha]_D^{21}$ +99.6 (c, 1.8 in MeOH). Formerly given a struct. with the oxazole ring in open-form under the name Parabactin A. λ_{max} 250 (ϵ 26600); 310 (ϵ 11000) (EtOH) (Berdy). λ_{max} 208 (ϵ 50000); 310 (ϵ 7700) (pH 7 buffer) (Berdy). λ_{max} 210 (ϵ 56800); 253 (ϵ 27300); 319 (ϵ 8200) (pH 1.5 buffer) (Berdy).

[54135-85-2]

Tait, G.H. *et al., Biochem. J.*, 1975, **146**, 191 (*Parabactin*)
Ong, S.A. *et al., J. Biol. Chem.*, 1979, **254**, 1860 (*isol, props*)
Sciortino, C.V. *et al., J. Lab. Clin. Med.*, 1980, **96**, 1081 (*props*)
Peterson, T. *et al., J.A.C.S.*, 1980, **102**, 7715 (*synth, struct*)
Eng-Wilmot, D.L. *et al., J.A.C.S.*, 1980, **102**, 7719 (*cryst struct*)
Neilands, J.B. *et al., Methods Enzymol.*, 1983, 94 (*rev*)
Bergeron, R.J. *et al., Biochem. Biophys. Res. Commun.*, 1984, **121**, 848 (*activity*)
Nagao, Y. *et al., J.C.S. Perkin 1*, 1984, 183 (*Parabactin*)
Bergeron, R.J. *et al., J.O.C.*, 1985, **50**, 2780 (*synth*)
Bergeron, R.J. *et al., Cancer Res.*, 1987, **47**, 6010 (*Parabactin, pharmacol*)
Bergeron, R. *et al., Blood*, 1993, **82**, 2552 (*Parabactin, pharmacol*)

Agrochelin **A-204**

[247115-74-8]

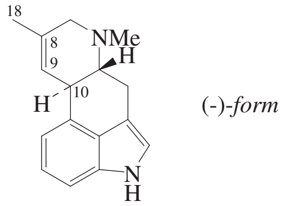


$C_{23}H_{34}N_2O_4S_2$ 466.665
Alkaloid from a marine *Agrobacterium* sp. Cytotoxic agent. Siderophore. Pale yellow oil. $[\alpha]_D^{25}$ -20.5 (c, 0.2 in $CHCl_3$). Chelates $Zn^{2\oplus}$ ion. λ_{max} 210 (log ϵ 5.18); 264 (log ϵ 4.8) (MeOH).

Acebal, C. *et al., J. Antibiot.*, 1999, **52**, 983-987 (*isol*)
Canedo, L.M. *et al., Tet. Lett.*, 1999, **40**, 6841-6844 (*isol, uv, cd, pmr, cmr*)

Agroclavine **A-205**

8,9-Didehydro-6,8-dimethylergoline, 9CI



$C_{16}H_{18}N_2$ 238.332

(-)-form [548-42-5]
Alkaloid from ergot and from several spp. in the genera *Argyreia*, *Rivea*, *Cuscuta*, *Ipomoea* (Convolvulaceae). Prod. by *Penicillium* , *Aspergillus* and *Rhizopus* spp. CNS excitator acting by stimulation of sympathetic centres. Active against gram-positive bacteria. Mycotoxin. Sol. MeOH, $CHCl_3$, Py; fairly sol. C_6H_6; poorly sol. H_2O. Mp 208-209° dec. $[\alpha]_D$ -151 ($CHCl_3$). $[\alpha]_D$ -182 (Py). λ_{max} 225 (ϵ 29512); 284 (ϵ 7586); 293 (ϵ 6456) (MeOH) (Berdy).
▸ LD_{50} (mus, ipr) 25 mg/kg. KE6325000

Dihydro: see Festuclavine, F-49

18-Hydroxy: **Elymoclavine**
[548-43-6]
$C_{16}H_{18}N_2O$ 254.331
Alkaloid from ergot and several other *Claviceps* spp. and from *Stictocardia tiliaefolia*, *Stictocardia campanulata*, *Argyreia* spp. and several other spp.in the Convolvulaceae. Prod. by *Penicillium aurantiovirens.* 5HT receptor antagonist. CNS excitatory agent acting by stimulation of sympathetic centres. Mycotoxin. Sol. MeOH, $CHCl_3$; fairly sol. C_6H_6; poorly sol. H_2O. Mp 250-252° dec. $[\alpha]_D$ -152 (c, 1 in Py). λ_{max} 227 (ε 20417); 283 (ε 6918); 293 (ε 5754) (MeOH) (Berdy).

▶ KE6340000

18-Hydroxy, O-*β*-D-*fructofuranoside:* *Elymoclavine* O-*β*-D-*fructofuranoside*
[28986-92-7]
[121844-72-2]
$C_{22}H_{28}N_2O_6$ 416.473
Isol. from the *Claviceps* strain SD 58 grown in a culture medium containing saccharose. Amorph. Prob. artifact formed in a secondary process from Elymoclavine and fructose from saccharose in the culture medium.

18-Hydroxy, O-*[β*-D-*fructofuranosyl-(2→1)-β*-D-*fructofuranoside]: Elymoclavine* O-*β*-D-*fructofuranosyl-(2→1)-*O-*β*-D-*fructofuranoside*
[121864-94-6]
$C_{28}H_{38}N_2O_{11}$ 578.615
Isol. from saprophytic cultures of *Claviceps* strain SD 58 and *Claviceps purpurea* strain 88 EP on sucrose medium.

18-Hydroxy, O-*4-nitrobenzoyl:* Mp 176-177° dec. $[\alpha]^{20}_{D}$ -127 (c, 0.4 in $CHCl_3$).

*18-Hydroxy, 5,10-didehydro: 4,6,7,8-Tetrahydro-7-methylindolo[4,3-*fg*]quinoline-9-methanol.* **Dehydroelymoclavine**
[141869-64-9]
$C_{16}H_{16}N_2O$ 252.315
Alkaloid from roots of *Securidaca longipedunculata*.

10-Epimer: ***Agroclavine I***
[82597-81-7]
$C_{16}H_{18}N_2$ 238.332
Metab. of *Penicillium kapuscinskii* strain UCM F-2156D. λ_{max} 211 (sh) (ε 14600); 225 (ε 25500); 276 (sh) (ε); 282 (ε 5470); 292 (ε 4560) (MeOH) (Derep).

10-Epimer, N*¹-methoxy:* ***1-Methoxyagroclavine I***
[207349-44-8]
$C_{17}H_{20}N_2O$ 268.358
Prod. by *Penicillium* sp. WC75209. Inhibitor of Lck tyrosine kinase. $[\alpha]_D$ -63 (c, 0.08 in MeOH). λ_{max} 228 ; 282 (MeOH).

10-Epimer, 8β,9β-epoxide: ***Epoxyagroclavine I***
[82564-34-9]
$C_{16}H_{18}N_2O$ 254.331
Metab. from *Penicillium kapuscinskii* and *Penicillium sizovae* VKM.F1073. Mycotoxin. λ_{max} 211 (sh) (ε 14600); 225 (ε 25500); 276 (sh) (ε); 282 (ε 5470); 292 (ε 4560) (MeOH) (Derep).

(±)-form
Synthetic. Mp 189-191° dec.

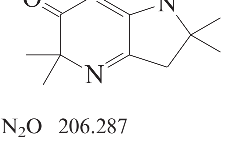
*18-Hydroxy:*Synthetic. Cryst. ($CHCl_3$/MeOH). Mp 207-210° dec.

10-Epimer: Synthetic.
Cryst. (Et_2O). Mp 157-158° (152-154°).

Stoll, A. *et al., Helv. Chim. Acta*, 1954, **37**, 1815-1825 (*Elymoclavine, isol, uv*)
Schreier, E. *et al., Helv. Chim. Acta*, 1958, **41**, 1984-1997 (*Elymoclavine, config*)
Floss, H.G. *et al., Z. Naturforsch., B*, 1967, **22**, 399-402 (*Elymoclavin fructoside*)
Inoue, T. *et al., Chem. Pharm. Bull.*, 1972, **20**, 409-411 (*ms*)
Chao, J.-M. *et al., Phytochemistry*, 1973, **12**, 2435-2440 (*occur*)
Bach, N.J. *et al., J.O.C.*, 1974, **39**, 1272-1276 (*pmr, cmr*)
Maier, W. *et al., Biochem. Physiol. Pflanz.*, 1978, **172**, 531-536 (*biosynth*)
Wurst, M. *et al., J. Chromatogr.*, 1978, **150**, 477; 1979, **174**, 401-407 (*hplc*)
Mrtek, R.G. *et al., Phytochemistry*, 1978, **7**, 1535 (*Elymoclavine, pmr*)
Saini, M. *et al., Phytochemistry*, 1978, **17**, 799 (*biosynth*)
Kiguchi, T. *et al., Heterocycles*, 1984, **22**, 43-45; 1985, **23**, 2891-2893 (*Agroclavine I, synth*)
Sakharovsky, V.G. *et al., Tet. Lett.*, 1984, **25**, 109-112 (*Agroclavine I, Epoxyagroclavine I*)
Eich, E. *et al., Arzneim.-Forsch.*, 1985, **35**, 1760-1762 (*activity*)
Kozikowski, A.P. *et al., J.A.C.S.*, 1985, **107**, 2569-2571 (*Agroclavine I, synth*)
Somei, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 948-950 (*synth*)
Wheeler, W.J. *et al., Tet. Lett.*, 1986, **27**, 3469-3470 (*synth*)
Somei, M. *et al., Heterocycles*, 1987, **26**, 895-898; 1997, **45**, 1263-1266 (*Agroclavine I, synth*)
Flieger, M. *et al., J. Nat. Prod.*, 1989, **52**, 506-510; 1991, **54**, 390-395 (*cmr, Elymoclavine fructosides*)
Ninomiya, I. *et al., Chem. Pharm. Bull.*, 1991, **39**, 23-30 (*Agroclavine I, synth*)
Costa, C. *et al., J. Het. Chem.*, 1992, **29**, 1641-1647 (*Dehydroelymoclavine*)
Padmanabha, R. *et al., Bioorg. Med. Chem. Lett.*, 1998, **8**, 569-574 (*1-Methoxyagroclavine*)
Yamada, F. *et al., Heterocycles*, 2007, **72**, 599-620 (*Agroclavine I, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, AEY375; EAJ000 (*Agroclavine, Elymoclavine*)

Agrocybenine A-206

*1,2,3,5-Tetrahydro-2,2,5,5,7-pentamethyl-6*H*-pyrrolo[2,3-*b*]pyridin-6-one, 9CI*
[178764-92-6]

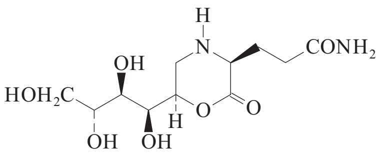


$C_{12}H_{18}N_2O$ 206.287
Alkaloid from the edible Korean mushroom yangimatusutake (*Agrocybe cylindracea*). Prolyl endopeptidase inhibitor. Mycotoxin. Yellow powder. λ_{max} 223 (ε 16800); 333 (ε 9200) (MeOH).

Koshino, H. *et al., Tet. Lett.*, 1996, **37**, 4549 (*isol, uv, ir, pmr, cmr, N-15 nmr, struct*)

Agropine A-207

2-Oxo-6-(1,2,3,4-tetrahydroxybutyl)-3-morpholinepropanamide, 9CI
[70699-77-3]

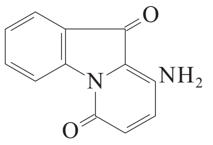


$C_{11}H_{20}N_2O_7$ 292.288
Struct. revised in 1982. Obt. from crown gall tumours.

Coxon, D.T. *et al., Tet. Lett.*, 1980, 495 (*synth, spectra*)
Tate, M.E. *et al., Carbohydr. Res.*, 1982, **104**, 105 (*ms, struct*)
Chilton, W.S. *et al., Phytochemistry*, 1995, **40**, 619 (*occur*)

Ailanindole A-208

*9-Aminopyrido[1,2-*a*]indole-6,10-dione, 9CI*
[159903-51-2]

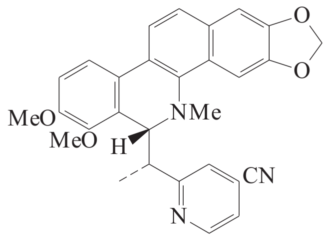


$C_{12}H_8N_2O_2$ 212.207
Alkaloid from the wood of *Ailanthus malabarica*. Orange needles (MeOH). Mp 300°. Intense green fluorescence in org. solvs. λ_{max} 238 (log ε 4.16); 252 (sh) (log ε 3.97); 296 (sh) (log ε 3.33); 452 (log ε 3.83); 474 (log ε 3.82) (MeOH).

Aono, H. *et al., Phytochemistry*, 1994, **37**, 579-584 (*isol, uv, ir, pmr, cmr, ms*)

Ailanthoidine A-209

[86003-22-7]

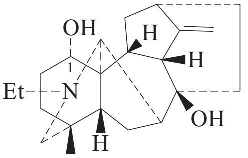


$C_{29}H_{25}N_3O_4$ 479.534
Alkaloid from the bark of *Zanthoxylum ailanthoides* (Rutaceae). Mp 260-263°. $[\alpha]_D$ 0.

Ishii, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1340 (*isol, pmr, cmr, cryst struct*)

Ajabicine A-210

[148225-24-5]



$C_{22}H_{33}NO_2$ 343.508

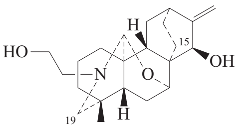
Unique methyleneaconitane struct. Alkaloid from leaves of *Delphinium ajacis* (Ranunculaceae). Amorph.

1-Ketone: ***Actaline***
[122279-81-6]
$C_{22}H_{31}NO_2$ 341.492
Alkaloid from the epigeal part of *Aconitum talassicum* (Ranunculaceae). Cryst. (hexane). Mp 125-127°.

Nishanov, A.A. *et al., Khim. Prir. Soedin.*, 1989, **25**, 39; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 32 (*isol, ir, pmr, ms, cryst struct*)
Joshi, B.S. *et al., Tet. Lett.*, 1993, **34**, 1441 (*isol, pmr, cmr, struct*)

Ajaconine, 9CI A-211

[545-61-9]



Absolute configuration

$C_{22}H_{33}NO_3$ 359.508

Alkaloid from *Delphinium virescens* and *Delphinium carolinianum* (whole plants), the roots of *Delphinium tatsienense*, and the seeds of *Delphinium consolida, Delphinium ajacis* and *Consolida ambigua* (Ranunculaceae). Also isol. from *Consolida oliveriana*. Mp 167°. $[\alpha]_D$ -122 (c, 1.75 in EtOH). pK_{a1} 11.8 (50% MeOH aq.). pK_{a1} 11.3 (80% EtOH aq.).

Sulfate (2:1):
Cryst. + 7H_2O (Me_2CO aq.). Mp 113° (hydrate) Mp 231° (anhyd.).

15-Epimer: ***15-Epiajaconine***. *Deacetylspiramine F*
$C_{22}H_{33}NO_3$ 359.508
Alkaloid from *Spiraea japonica* var. *ovalifolia*. Plates (Me_2CO). Mp 149-151°.

15-Epimer, 15-Ac: ***Spiramine F***
[142750-37-6]
$C_{24}H_{35}NO_4$ 401.545
Alkaloid from roots of *Spiraea japonica* var. *acuminata* (Rosaceae). Amorph. $[\alpha]_D^{18}$ -101 (c, 2.5 in $CHCl_3$).

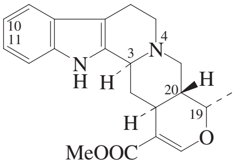
15-Epimer, di-Ac: ***Spiramine E***
[142750-36-5]
$C_{26}H_{37}NO_5$ 443.582
Alkaloid from roots of *Spiraea japonica* var. *acuminata* (Rosaceae). Amorph. $[\alpha]_D^{20}$ -97 (c, 1.9 in $CHCl_3$).

15-Epimer, 19-oxo, 15-Ac: ***Spiramine R***
[162858-00-6]
$C_{24}H_{33}NO_5$ 415.528
Alkaloid from roots of *Spiraea japonica* var. *incisa* (Rosaceae). Needles (EtOAc). Mp 190-192°. $[\alpha]_D$ -180 (c, 0.39 in $CHCl_3$).

Keller, O. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1913, **251**, 207; *CA*, **8**, 674 (*isol*)
Dvornik, D. *et al., Tetrahedron*, 1961, **14**, 54 (*isol, ir, struct*)
Scott, A.I. *et al., Tetrahedron*, 1971, **27**, 4787 (*cd*)
Sastry, S.D. *et al., Chem. Ind. (London)*, 1972, 381 (*ms*)
Pelletier, S.W. *et al., Heterocycles*, 1979, **12**, 779; 1981, **16**, 747; 1983, **20**, 1347 (*occur*)
Pelletier, S.W. *et al., J. Nat. Prod.*, 1980, **43**, 395 (*isol, ir, pmr*)
Hao, X.-J. *et al., Heterocycles*, 1993, **36**, 825 (*Spiramine E, Spiramine F*)
Hao, X.-J. *et al., Phytochemistry*, 1995, **38**, 545 (*Spiramine R*)
Ulubelen, A. *et al., J. Nat. Prod.*, 1996, **59**, 907 (*cmr*)
Zuo, G.Y. *et al., Heterocycles*, 2001, **55**, 487-493 (*15-Epiajaconine*)
González-Coloma, A. *et al., Chem. Biodiversity*, 2004, **1**, 1327-1335 (*isol, pmr*)

Ajmalicine A-212

Methyl 16,17-didehydro-19-methyloxayohimban-16-carboxylate, 9CI. Tetrahydroserpentine. Raubasine. δ-Yohimbine. Vinceine. Vincaine†. Py-tetrahydroserpentine. Lamuran



Absolute Configuration

$C_{21}H_{24}N_2O_3$ 352.432
Log P 2.76 (calc).

(-)-form [483-04-5]
Alkaloid from *Rauwolfia serpentina*, many other *Rauwolfia* spp., *Catharanthus roseus* and many other spp. in the Apocynaceae. Antidiuretic agent, CNS depressant. Vasodilator. Has been used to treat peripheral and cerebral vascular disorders. Active against fungi. Prisms (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 259° dec. $[\alpha]_D$ -66 ($CHCl_3$). λ_{max} 227 (ϵ 40740); 246 (sh) (ϵ 11750); 280 (ϵ 6920); 292 (ϵ 6160) (MeOH) (Berdy).

▶ LD_{50} (mus, orl) 400 mg/kg. Human systemic effects by ingestion. AX7875000

Hydrochloride:
Leaflets (EtOH). Mp 289°. $[\alpha]_D^{20}$ -17 (c, 0.5 in MeOH).

3-Epimer: ***3-Isoajmalicine***
[483-03-4]
$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from *Mitragyna* and *Uncaria* spp. (Rubiaceae). Needles (Et_2O). Mp 193-194°. λ_{max} 225 (log ϵ 4.61); 250 (log ϵ 4.14); 282 (log ϵ 3.93); 291 (log ϵ 3.87) (EtOH).

19-Epimer: ***Mayumbine***. *19-Epiajmalicine*
[25532-45-0]
$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from *Pseudocinchona mayumbensis* (syn. *Corynanthe mayumbensis*), *Uncaria elliptica* and *Rauwolfia yunnanensis* (Rubiaceae, Rubiaceae, Apocynaceae). Mp 216°. $[\alpha]_D$ -68 (Py). λ_{max} 227 (log ϵ 4.6); 280 (log ϵ 3.84); 292 (log ϵ 3.8) (MeOH).

19-Epimer, hydrochloride: Mp 293-294°. $[\alpha]_D^{20}$ -96 (MeOH).

19-Epimer, 20,21-didehydro: see Cathenamine, C-207

20-Epimer: ***Tetrahydroalstonine***
[6474-90-4]
$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from *Alstonia*, *Amsonia*, *Cabucala*, *Catharanthus*, *Mitragyna*, *Rauwolfia*, *Uncaria*, *Rhazya* and *Voacanga* spp. Active against gram-positive bacteria. Lustrous plates (EtOH aq.). Mp 230-231°. $[\alpha]_D^{27}$ -108 (c, 0.5 in $CHCl_3$). λ_{max} 226 (log ϵ 4.64); 248 (sh) (log ϵ 4.07); 272 (log ϵ 3.78); 280 (sh) (log ϵ 3.85); 291 (log ϵ 3.83) (MeOH) (Berdy).

20-Epimer, N^b*-oxide(*R*-):* ***Tetrahydroalstonine (4R)-N-oxide***
[41590-28-7]
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from *Uncaria* spp. (Rubiaceae). Cryst. (Me_2CO/Et_2O). Mp 172-174° dec. $[\alpha]_D^{20}$ +33.8 (c, 0.11 in MeOH). λ_{max} 224 (ϵ 43400); 245 (sh) (ϵ 11800); 273 (sh) (ϵ 7100); 282 (ϵ 7450); 290 (ϵ 6400) (EtOH).

20-Epimer, N^b*-Me:* ***Melinonine A***. N^b*-Methyltetrahydroalstonine*
[6801-41-8]
$C_{22}H_{27}N_2O_3^{\oplus}$ 367.467
Quaternary alkaloid from *Strychnos melinoniana* and *Rauwolfia volkensii* (Loganiaceae, Apocynaceae). Hygroscopic needles (EtOH/Me_2CO) (as chloride). Mp 260-261° (chloride). $[\alpha]_D^{20}$ -120 (H_2O) (chloride). λ_{max} 225 (log ϵ 4.8); 279 (log ϵ 4); 290 (log ϵ 3.8) (MeOH).

3,19-Diepimer: ***19-Epi-3-isoajmalicine***
[25532-46-1]
$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from *Uncaria elliptica, Uncaria attenuata* and *Catharanthus roseus* (Rubiaceae, Apocynaceae). λ_{max} 225 ; 273 (sh) ; 283 ; 290 (MeOH).

3,20-Diepimer: ***Akuammigine***
[642-17-1]
$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from *Picralima nitida (Picralima klaineana)* and some *Uncaria* spp. (Apocynaceae, Rubiaceae). Mp 125° (113°). $[\alpha]_D^{20}$ -44.4 (EtOH). $[\alpha]_D^{18.5}$ -42 (c, 1.6 in EtOH).

3,20-Diepimer, hydrochloride: Mp 287°. $[\alpha]_D^{20}$ -38 (MeOH).

*3,20-Diepimer, (4*R*)-*N*-oxide:* ***Akuammigine (4R)-N-oxide***
[41590-26-5]
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from an *Uncaria* sp. Cryst. (Me_2CO/Et_2O). Mp 214-215°. $[\alpha]_D^{20}$ -20 (c, 0.11 in MeOH). $[\alpha]_D^{20}$ -46 (c, 0.41 in Py). λ_{max} 223 (ϵ 43000); 245 (sh) (ϵ 13150); 281 (ϵ 8300); 291 (ϵ 6600) (EtOH).

*3,20-Diepimer, (4*S*)-*N*-oxide:* ***Akuammigine (4S)-N-oxide***

[41590-27-6]
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from an *Uncaria* sp. (Rubiaceae). Cryst. (Me_2CO/Et_2O). Mp 195-197° dec. $[\alpha]_D^{20}$ -112 (c, 0.12 in MeOH). λ_{max} 224 (ϵ 43400); 246 (sh) (ϵ 10200); 273 (sh) (ϵ 7900); 282 (ϵ 8350); 290 (ϵ 7150) (EtOH).

19,20-Diepimer: ***Rauniticine***. *Ervine*†
[5299-09-2]
$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from *Rauwolfia nitida, Uncaria elliptica, Uncaria attenuata, Vinca libanotica, Vinca major* and *Veratrum album lobelianum* (Apocynaceae, Rubiaceae, Liliaceae). Cryst. (MeOH). Mp 233-235°. $[\alpha]_D$ -6.6 (Py). $[\alpha]_D$ -38.4 ($CHCl_3$). λ_{max} 228 (log ϵ 4.65); 246 (sh) (log ϵ 4.09); 282 (log ϵ 3.91); 288 (log ϵ 3.79) (EtOH).

19,20-Diepimer, 14α-hydroxy: ***14α-Hydroxyrauniticine***
[77101-58-7]
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from the leaves of *Uncaria attenuata* and *Uncaria elliptica* (Rubiaceae). Plates (MeOH). Mp 174-175° dec. $[\alpha]_D$ -17.5 (c, 0.1 in MeOH). Originally proposed as 14β-Hydroxy-3-isorauniticine.

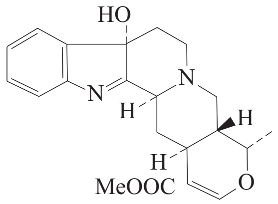
3,19,20-Triepimer: ***3-Isorauniticine***
[6870-40-2]
$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from *Corynanthe mayumbensis* and the leaves of *Uncaria elliptica* (Apocynaceae, Rubiaceae). Cryst. + $^1/_2$ H_2O (as hydrochloride). Mp 277° (hydrochloride). $[\alpha]_D$ +25 (c, 1 in MeOH) (as hydrochloride).

(±)*-form* [24196-16-5]
Synthetic. Mp 228-231°.
Hydrochloride: Mp 285-286° dec.
3,20-Diepimer: [20361-85-7]
Synthetic. Mp 143° (125-126°).

Henry, T.A. *et al., J.C.S.*, 1932, 2759-2768 (*Akuammigine, isol*)
Schlittler, E. *et al., Helv. Chim. Acta*, 1952, **35**, 29-45 (*Melinonine A*)
Klohs, M.W. *et al., J.A.C.S.*, 1954, **76**, 1332-1334 (*isol, uv, ir*)
Robinson, R. *et al., J.C.S.*, 1954, 3479-3482 (*Akuammigine, isol, uv, ir, struct*)
Raymond-Hamet, *et al., C. R. Hebd. Seances Acad. Sci.*, 1961, **253**, 2776-2778 (*Akuammigine, pharmacol*)
Salkin, R. *et al., J. Pharm. Sci.*, 1961, **50**, 1038-1041 (*Rauniticine, isol, uv, ir, struct*)
Antonaccio, L.D. *et al., J.A.C.S.*, 1962, **84**, 2161-2169 (*ms*)
Shamma, M. *et al., J.A.C.S.*, 1963, **85**, 2507-2512 (*ir, pmr, config*)
Hesse, M. *et al., Helv. Chim. Acta*, 1965, **48**, 674-689 (*Melinonine A, ms*)
Finch, N. *et al., Tetrahedron*, 1966, **22**, 1327-1333 (*Rauniticine, uv, ord, stereochem*)
Laubie, M. *et al., Arzneim.-Forsch.*, 1969, **19**, 1820-1826 (*pharmacol*)
Winterfeld, E. *et al., Chem. Ber.*, 1969, **102**, 3558-3572 (*epimer, synth*)
Van Tamelen, E.E. *et al., J.A.C.S.*, 1969, **91**, 7359-7371 (*synth*)
Gutzwiller, J. *et al., J.A.C.S.*, 1971, **93**, 5907-5908 (*synth, ir, ms, pmr, Akuammigine*)
Merlini, L. *et al., Tetrahedron*, 1972, **28**, 5971-5975 (*Akuammigine oxides, Tetrahydroalstonine oxide, isol, synth*)
Levin, R.H. *et al., J.O.C.*, 1973, **38**, 1983-1992 (*cmr*)
Lohr, J.P. *et al., Arzneim.-Forsch.*, 1975, **25**, 870-873 (*metab*)
Wenkert, E. *et al., J.A.C.S.*, 1976, **98**, 3645-3655 (*Akuammigine, Tetrahydroalstonine, synth, cmr*)
Brown, R.T. *et al., J.C.S. Perkin 1*, 1976, 160-162 (*Mayumbine, Tetrahydroalstonine, synth*)
Brown, R.T. *et al., Chem. Comm.*, 1977, 636-638 (*synth, Akuammigine, Tetrahydroalstonine*)
Melchio, J. *et al., Tet. Lett.*, 1977, 315-316 (*Mayumbine, 3-Isorauniticine, bibl, config*)
Sakai, S. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2596-2598 (*Akuammigine, 3-Isorauniticine, synth*)
Stöckigt, J. *et al., Phytochemistry*, 1979, **18**, 965-971 (*biosynth*)
Akinloye, B.A. *et al., Phytochemistry*, 1980, **19**, 307-311 (*Melinonine A*)
Ponglux, D. *et al., Phytochemistry*, 1980, **19**, 2013-2016 (*Rauniticine, isol, uv, ir, ms*)
Gutzwiller, J. *et al., Helv. Chim. Acta*, 1981, **64**, 1663-1671 (*synth*)
Wenkert, E. *et al., Acta Chem. Scand., Ser. B*, 1982, **36**, 607-611 (*stereochem, config*)
Kohl, W. *et al., Z. Naturforsch., B*, 1982, **37**, 1346-1351 (*3,19-diepimer, isol, uv, pmr, ms*)
Seguin, E. *et al., Helv. Chim. Acta*, 1983, **66**, 2059-2068 (*cd*)
Phillipson, J.D. *et al., Phytochemistry*, 1983, **22**, 1809-1813 (*3-Isorauniticine, Rauniticine, 3,19-diepimer, Tetrahydroalstonine N-oxide, isol*)
Massiot, G. *et al., Chem. Comm.*, 1984, 715-716 (*synth*)
Lala, P.K. *et al., J. Inst. Chem. (India)*, 1984, **56**, 42-47 (*ms*)
Palmisano, G. *et al., J.C.S. Perkin 1*, 1985, 923-926 (*19-Epiajmalicine, Mayumbine, synth, uv, ir, pmr, ms*)
Hatakeyama, S. *et al., Tet. Lett.*, 1985, **26**, 865-868 (*synth*)
Yamanaka, E. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3713-3721 (*14α-Hydroxyrauniticine, synth, pmr*)
Naito, T. *et al., Heterocycles*, 1986, **24**, 2117-2120 (*synth*)
Mekkawi, A.G. *et al., Anal. Profiles Drug Subst.*, 1987, **16**, 731 (*rev*)
Morales-Rios, M.S. *et al., Magn. Reson. Chem.*, 1987, **25**, 377-395 (*cmr*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 6133
Takano, S. *et al., Chem. Comm.*, 1988, 59-60 (*synth, Tetrahydroalstonine*)
Hirai, Y. *et al., J.A.C.S.*, 1988, **110**, 958-960 (*synth, Tetrahydroalstonine*)
Martin, S.F. *et al., J.A.C.S.*, 1988, **110**, 5925-5927 (*Tetrahydroalstonine, synth, bibl*)
Baggiolini, E.G. *et al., Tetrahedron*, 1988, **44**, 3203-3208 (*19-Epiajmalicine, Mayumbine, synth, ir, pmr, ms*)
Oppolzer, W. *et al., J.A.C.S.*, 1991, **113**, 9660-9661 (*3-Isorauniticine, synth*)
Hanessian, S. *et al., J.O.C.*, 1991, **56**, 2947-2949 (*19-Epiajmalicine, Mayumbine, synth*)
Honda, T. *et al., J.C.S. Perkin 1*, 1993, 539-540 (*19-Epiajmalicine, Mayumbine, synth*)
Lögers, M. *et al., J.A.C.S.*, 1995, **117**, 9139-9150 (*synth*)
Arbain, D. *et al., Aust. J. Chem.*, 1998, **51**, 961-964 (*Rauniticine, 14-Hydroxyrauniticine, isol, pmr, cryst struct*)
Laus, G. *et al., Helv. Chim. Acta*, 2008, **91**, 831-837 (*Akuammigine, cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, AFG750

Ajmalicine hydroxyindolenine A-213

[5802-03-9]

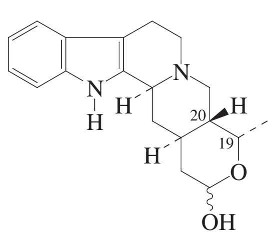


$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from *Catharanthus roseus* tissue culture (Apocynaceae).

Guéritte, F. *et al., J. Nat. Prod.*, 1983, **46**, 144-148 (*isol*)

Ajmalicinial A-214

[81737-77-1]



$C_{19}H_{24}N_2O_2$ 312.411
Alkaloid from *Strychnos johnsonii*. No phys. props. reported.

N^1-Methoxycarbonyl: ***Ajmalicidine***
[109031-00-7]
$C_{21}H_{26}N_2O_4$ 370.447
Alkaloid from the roots of *Rauwolfia serpentina* (Apocynaceae). Plates (MeOH/EtOAc). Mp 235-236°. $[\alpha]_D^{20}$ +190 ($CHCl_3$). The struct. assigned is prob. incorrect. Proposed by Lounasmaa *et al* to be possibly identical with Ajmalicinine, A-215. λ_{max} 208 ; 225 ; 285 (no solvent reported).

N^1-Methoxycarbonyl, Ac: [109031-01-8]
Needles. Mp 251-252°.

20-Epimer: ***Tetrahydroalstonial***
[85717-32-4]
$C_{19}H_{24}N_2O_2$ 312.411
Alkaloid from *Strychnos johnsonii*. No phys. props. reported.

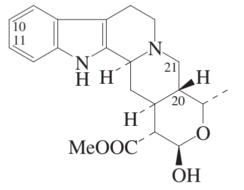
Stereoisomer (?): ***16-Descarbomethoxy-16,17-dihydro-17-hydroxy-19-epiajmalicine***
[78184-81-3]
$C_{19}H_{24}N_2O_2$ 312.411
Alkaloid from the bark of *Hunteria zeylanica* and the root bark of *Aspidosperma marcgravianum* (Apocynaceae). Mp 185°. $[\alpha]_D$ -86 (Py). Stereochem. unclear. Shown in both papers as having same 19-config. as Ajmalicine, but both papers refer to it as an 19-epiajmalicine. May be identical with Ajmalicinial.

Arambewela, L.S.R. *et al., Phytochemistry*, 1981, **20**, 349-350 (*Descarbomethoxydihydrohydroxyepiajmalicine*)

Chatterjee, A. *et al., J.O.C.*, 1982, **47**, 3113-3117 (*synth, pmr*)
Robert, G.M.T. *et al., J. Nat. Prod.*, 1983, **46**, 694-707 (*Descarbomethoxydihydrohydroxyepiajmalicine*)
Palmisano, G. *et al., J.C.S. Perkin 1*, 1985, 923-926 (*synth, pmr, ms*)
Siddiqui, S. *et al., Phytochemistry*, 1987, **26**, 875-877 (*Ajmalicidine*)
Massiot, G. *et al., Phytochemistry*, 1987, **26**, 2839-2846 (*Ajmalicinial, Tetrahydroalstonial*)
Lounasmaa, M. *et al., Planta Med.*, 1994, **60**, 480-481 (*Ajmalicidine*)

Ajmalicinine A-215

[55529-55-0]



Absolute Configuration

$C_{21}H_{26}N_2O_4$ 370.447
Alkaloid from the root bark of *Cabucala striolata* and the stem bark of *Rauwolfia cumminsii* and *Rauwolfia caffra* (Apocynaceae).

11-Methoxy: ***Tetraphyllinine***
[23924-91-6]
$C_{22}H_{28}N_2O_5$ 400.474
Alkaloid from *Rauwolfia discolor* and from the leaves of *Neisosperma glomerata* (Apocynaceae). Plates (MeOH). Mp 231-234°. $[\alpha]_D^{20}$ -35 (c, 0.42 in Py).

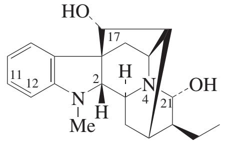
10,11-Dimethoxy: ***10,11-Dimethoxyajmalicinine***
[55511-11-0]
$C_{23}H_{30}N_2O_6$ 430.5
Alkaloid from the root bark of *Cabucala striolata* and the trunk bark of *Ochrosia moorei* (Apocynaceae).

Stereoisomer, 20,21-didehydro: ***16,17-Dihydro-17-hydroxy-19-epicathenamine***
[69284-02-2]
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from *Guettarda eximia* (Rubiaceae). Isol. as an inseparable mixt. of two epimers at C-16 and/or C-17. Not named in the original papers.

Winternitz, F. *et al., Phytochemistry*, 1969, **8**, 1797-1802 (*Tetraphyllinine, synth, pmr, abs config*)
Bombardelli, E. *et al., Fitoterapia*, 1974, **45**, 183-187; *CA*, **83**, 25051u (*Ajmalicinine, Dimethoxyajmalicinine, isol, struct*)
Kan-Fan, C. *et al., Chem. Comm.*, 1978, 618-619 (*16,17-Dihydro-17-hydroxy-19-epicathenamine*)
Iwu, M.M. *et al., Phytochemistry*, 1978, **17**, 1651-1654 (*isol*)
Brown, R.T. *et al., Chem. Comm.*, 1979, 877-879 (*16,17-Dihydro-17-hydroxy-19-epicathenamine, synth*)
Ahond, A. *et al., J. Nat. Prod.*, 1981, **44**, 193-199 (*Dimethoxyajmalicinine*)
Seguin, E. *et al., J. Nat. Prod.*, 1982, **45**, 738-744 (*Tetraphyllinine, isol*)
Seguin, E. *et al., Helv. Chim. Acta*, 1983, **66**, 2059-2068 (*cd*)
Nasser, A.M.A.G. *et al., J. Ethnopharmacol.*, 1984, **11**, 99-117; *CA*, **102**, 3224m (*isol*)

Ajmaline, BAN, JAN A-216

Ajmalan-17,21-diol, 9CI. Ajimaline. Gilurytmal. Merabitol. Raugalline. Rauwolfine. Rytmalin. Tachmalin. Many other names
[4360-12-7]



Absolute Configuration

$C_{20}H_{26}N_2O_2$ 326.438
Alkaloid from *Rauwolfia serpentina* and most *Rauwolfia* spp., *Melodinus balansae* and *Tonduzia longifolia* (Apocynaceae). Antiarrhythmic (Class Ia) drug which functions by inhibition of glucose uptake by heart tissue mitochondria. Platelet activating factor antagonist. Antiinflammatory agent. Mp 158-160° (MeOH solvate) Mp 205-207° (anhyd.). $[\alpha]_D$ +144 ($CHCl_3$). Log P 1.26 (uncertain value) (calc).

▶ High doses may cause cardiac arrhythmias, coma and death. Adverse neurological, hepatic, and haematological effects also recorded. LD_{50} (rat, orl) 360 mg/kg. LD_{50} (rat, ipr) 94 mg/kg. AX8050000

Hydrochloride: [4410-48-4]
Amber prisms + $2H_2O$. Mp 133-134° Mp 253-255° (anhyd.).

▶ AX8100000

Hydrochloride (1:2):
Plates. Mp 305-306° dec.

Picrate:
Plates (EtOH). Mp 126-127° Mp 223° (anhyd.).

21-O-β-D-Glucopyranoside: ***Rauglucine***
[119365-83-2]
$C_{26}H_{36}N_2O_7$ 488.58
Alkaloid from *Rauwolfia serpentina* (Apocynaceae).

17-Ac: **17-O-*Acetylajmaline***
[19918-92-4]
$C_{22}H_{28}N_2O_3$ 368.475
Alkaloid from cell suspension cultures of *Rauwolfia serpentina*. Rods (Et_2O), cryst. (EtOH). Mp 150° (rods) Mp 214-215° (cryst.).

*17-Ac, 21-*O*-β-D-glucopyranoside:* ***Acetylrauglucine***
[119329-01-0]
$C_{28}H_{38}N_2O_8$ 530.617
Alkaloid from *Rauwolfia serpentina* (Apocynaceae). $[\alpha]_D^{20}$ +17 (c, 0.36 in EtOH).

21-Ac:
Needles (EtOAc). Mp 190-192°.

Di-Ac: [19775-56-5]
Needles (metastable) or rods. Mp 132° Mp 187-189° (double Mp).

*17-*O*-(3,4,5-Trimethoxybenzoyl):* ***Ajmalimine****. Willicourtine*
[59846-31-0]
[110941-51-0]
$C_{30}H_{36}N_2O_6$ 520.624
Alkaloid from *Rauwolfia obscura*, *Rauwolfia serpentina* and *Rauwolfia vomitoria* (Apocynaceae). Needles (MeOH/EtOAc). Mp 188-189°. $[\alpha]_D^{20}$ +105. Struct. of Ajmalimine revised in 2001.

*17-*O*-Chloroacetyl:* ***Lorajmine, INN***
[47562-08-3]
$C_{22}H_{27}ClN_2O_3$ 402.92
Cardiac depressant, antiarrhythmic agent. Cryst. Mp 232-235°. $[\alpha]_D$ +27.5 ($CHCl_3$). Log P 2.32 (uncertain value) (calc).

*17-*O*-Chloroacetyl; hydrochloride:* ***Lorajmine hydrochloride, USAN****. Nevergor. Ritmos. Ritmosel. Viaductor. Win 11831*
[40819-93-0]
Cryst. Mp 230-235°. $[\alpha]_D$ +40 ($CHCl_3$).

▶ LD_{50} (rat, orl) 480 mg/kg. LD_{50} (rat, ivn) 17.3 mg/kg. AX7710000

N^4*-Me:* **N^b-*Methylajmaline***
$C_{21}H_{29}N_2O_2^{\oplus}$ 341.472
Alkaloid from the roots of *Rauwolfia serpentina*. Amorph. powder (as chloride). $[\alpha]_D^{28}$ +113 (c, 1.1 in MeOH) (chloride). λ_{max} 205 (log ε 4.4); 244 (log ε 3.86); 288 (log ε 3.4) (MeOH) (chloride).

N^4*-Propyl, hydrogen tartrate:* ***Prajmalium bitartrate, BAN, INN****. Neorythmin. GT 1012. NPAB*
[2589-47-1]
$C_{27}H_{38}N_2O_8$ 518.606
Cardiac antiarrhythmic agent. Cryst. (EtOH/Et_2O). Mp 149-152°.

▶ LD_{50} (rat, orl) 54 mg/kg. LD_{50} (rat, ivn) 3.4 mg/kg. Hepatotoxic. AX7750000

N*-De-Me:* ***Norajmaline***
[23944-24-3]
$C_{19}H_{24}N_2O_2$ 312.411
Alkaloid from *Rauwolfia macrophylla, Rauwolfia obscura* and *Rauwolfia suaveolens* (Apocynaceae). Yellow-grey amorph. powder. $[\alpha]_D$ +36 (c, 0.67 in $CHCl_3$).

N*-De-Me, 17-Ac:* **17-O-*Acetylnorajmaline***
[80202-83-1]
$C_{21}H_{26}N_2O_3$ 354.448
Alkaloid from cell suspension cultures of *Rauwolfia serpentina*.

N*-De-Me, 17-Ac, 21-*O*-β-D-glucopyranoside:* ***Acetylnorrauglucine***
[119365-66-1]
$C_{27}H_{36}N_2O_8$ 516.59
Alkaloid from *Rauwolfia serpentina* (Apocynaceae).

17-Ketone: ***Ajmalidine***
[639-30-5]
$C_{20}H_{24}N_2O_2$ 324.422
Alkaloid from *Rauwolfia sellowii, Rauwolfia mauiensis* and *Rauwolfia vomitoria* (Apocynaceae). Prisms (MeOH). Mp 241-242°. $[\alpha]_D^{25}$ -80 (c, 1 in AcOH). pK_{a1} 6.3 (80% DMF). pK_{a1} 6.6 (60% DMF).

17-Ketone, O*-Ac:*
Needles (EtOH). Mp 218-220°. $[\alpha]_D^{25}$ +242 (c, 1 in Py).

11-Hydroxy: ***Ajmalinol***
[73012-74-5]
$C_{20}H_{26}N_2O_3$ 342.437
Alkaloid from *Rauwolfia vomitoria*

(Apocynaceae). Plates (C_6H_6/MeOH). Mp 209-210°. $[\alpha]_D^{30}$ +132 ($CHCl_3$). λ_{max} 254 ; 294 (no solvent reported).

12-Hydroxy: ***12-Hydroxyajmaline***
[152014-38-5]
$C_{20}H_{26}N_2O_3$ 342.437
Alkaloid from hairy roots of *Rauwolfia serpentina* (Apocynaceae). λ_{max} 250 ; 290 (MeOH).

12-Methoxy, 17-ketone: ***Vomalidine***
[639-28-1]
$C_{21}H_{26}N_2O_3$ 354.448
Alkaloid from the roots of *Rauwolfia vomitoria*, and root bark and stems of *Rauwolfia obscura* (Apocynaceae). Prisms (Me_2CO). Mp 242-243°. $[\alpha]_D^{20}$ +210 (c, 0.5 in Py). $[\alpha]_D$ +318 (c, 1 in $CHCl_3$).

12-Methoxy; 17-ketone, hydrochloride:
Cryst. (EtOH). Mp 239-242°.

12-Methoxy, 17-ketone, O*-Ac:*
Cryst. (Et_2O). Mp 252-254°. $[\alpha]_D^{20}$ +195 (c, 1 in Py).

2-Epimer: [51019-46-6]
Noncryst. $[\alpha]_D$ +55 (c, 1 in $CHCl_3$).

17-Epimer: ***Sandwicine****. Epiajmaline*
[509-37-5]
$C_{20}H_{26}N_2O_2$ 326.438
Alkaloid from *Rauwolfia sandwicensis, Rauwolfia mauiensis* and *Rauwolfia vomitoria* (Apocynaceae). Antiarrhythmic agent. Amorph. (MeOH aq. or Me_2CO/hexane). $[\alpha]_D^{20}$ +174 (c, 1 in MeOH).

17-Epimer; hydrochloride (1:2):
Cryst. (Me_2CO). Mp 210-213°. $[\alpha]_D$ +129 (MeOH).

17-Epimer, di-Ac:
Cryst. (petrol). Mp 105-108°. $[\alpha]_D^{20}$ +104 (c, 1 in $CHCl_3$).

20,21-Diepimer: ***Isoajmaline***
[6989-79-3]
$C_{20}H_{26}N_2O_2$ 326.438
Alkaloid from the roots of *Rauwolfia serpentina* (Apocynaceae). Prisms (MeOH aq.), plates (Et_2O). Mp 265° dec. $[\alpha]_D^{18}$ +72 (c, 0.7 in $CHCl_3$). pK_a 8.05.

20,21-Diepimer, hydrochloride (1:2):
Plates. Mp 310° dec.

20,21-Diepimer, di-Ac:
Plates (Et_2O). Mp 224-225°.

20,21-Diepimer, N^4*-Me:* **N^b-Methylisoajmaline**
$C_{21}H_{29}N_2O_2^{\oplus}$ 341.472
Alkaloid from the roots of *Rauwolfia serpentina*. Powder (as chloride). $[\alpha]_D^{21}$ +88 (c, 1.2 in MeOH) (chloride). λ_{max} 204 (log ϵ 4.41); 244 (log ϵ 3.88); 288 (log ϵ 3.42) (MeOH) (chloride).

17,20,21-Triepimer: ***Isosandwicine***
[6835-90-1]
$C_{20}H_{26}N_2O_2$ 326.438
Alkaloid from the roots of *Rauwolfia vomitoria* (Apocynaceae). Cryst. (MeOH aq.). Mp 250° (sinters at 160°). $[\alpha]_D^{20}$ +130 (c, 1.18 in $CHCl_3$).

17,20,21-Triepimer; hydrochloride: Mp 244-245°. $[\alpha]_D^{20}$ +133 (c, 1 in MeOH).

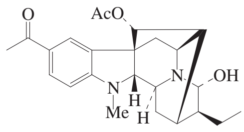
17,20,21-Triepimer, di-Ac:
Cryst. (EtOH aq.). Mp 160° (sinters at 110°). $[\alpha]_D^{20}$ +101 (c, 1 in $CHCl_3$).

[31081-68-2 , 35080-11-6 , 110906-81-5]

Anet, F.A.L. *et al., J.C.S.*, 1954, 1242-1260 (*isol, uv, struct, synth*)
Pakrashi, S.C. *et al., J.A.C.S.*, 1955, **77**, 6687-6689 (*Ajmalidine, isol, uv*)
Woodward, R.B. *et al., Angew. Chem.*, 1956, **68**, 13-20 (*rev, struct*)
Djerassi, C. *et al., J.A.C.S.*, 1956, **78**, 1259-1260 (*Ajmalidine, struct*)
Hofmann, A. *et al., Helv. Chim. Acta*, 1957, **40**, 1866-1874 (*Vomalidine*)
Gorman, M. *et al., Tetrahedron*, 1957, **1**, 328-337 (*Sandwicine*)
Bartlett, M.F. *et al., J.A.C.S.*, 1962, **84**, 622-630 (*abs config*)
Bonati, A. *et al., Farmaco, Ed. Sci.*, 1963, **18**, 851-863 (*Prajmalium, synth*)
Biemann, K. *et al., Tet. Lett.*, 1963, 1969-1973 (*Ajmalidine, ms*)
Keck, J. *et al., Z. Naturforsch., B*, 1963, **18**, 177-179 (*Prajmalium*)
Biemann, K. *et al., J.A.C.S.*, 1964, **86**, 4624-4628 (*Ajmaline, Vomalidine, ms*)
Albright, J.D. *et al., J.A.C.S.*, 1967, **89**, 2416-2423 (*Ajmalidine, synth, ir*)
Masamune, S. *et al., J.A.C.S.*, 1967, **89**, 2506-2509 (*synth*)
Mashimo, K. *et al., Tetrahedron*, 1970, **26**, 803-812 (*Isoajmaline, synth*)
Ronchetti, F. *et al., Phytochemistry*, 1971, **10**, 1385-1388 (*Sandwicine, Isosandwicine*)
Koch, M. *et al., Arzneim.-Forsch.*, 1972, **22**, 2079; 2085; 1973, **23**, 642 (*Prajmalium*)
Majumdar, S.P. *et al., Phytochemistry*, 1973, **12**, 1167-1169 (*Norajmaline*)
Petter, A. *et al., Arzneim.-Forsch.*, 1974, **24**, 873; 874; 876 (*rev, pharmacol, props*)
Timmins, P. *et al., Phytochemistry*, 1974, **13**, 281-282; 1997; 1976, **15**, 733-735 (*Norajmaline, Vomalidine*)
Hubert-Brierre, Y. *et al., Tetrahedron*, 1975, **31**, 3049-3054 (*synth, epimer*)
Kuhnert-Brandstaetter, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1976, **309**, 699-706 (*polymorphs*)
Van Tamelen, E.E. *et al., Bioorg. Chem.*, 1976, **5**, 309-326 (*synth*)
Timmins, P. *et al., Planta Med.*, 1976, **29**, 283-288 (*Ajmalimine*)
Prewo, R. *et al., Acta Cryst. B*, 1978, **34**, 454-460 (*cryst struct*)
Chatterjee, A. *et al., Tet. Lett.*, 1978, 3879-3882 (*cmr*)
Siddiqui, S. *et al., J. Chem. Soc. Pak.*, 1979, **1**, 1-4; *CA*, **92**, 111204p (*Ajmalinol, isol*)
Capra, C. *et al., Farmaco, Ed. Prat.*, 1980, **35**, 49-70 (*Lorajmine, pharmacol*)
Libot, F. *et al., Phytochemistry*, 1980, **19**, 989-991 (*Isoajmaline, cmr*)
Iwu, M.M. *et al., Planta Med.*, Suppl, 1980, 13 (*Ajmalimine*)
Stöckigt, J. *et al., Plant Cell Rep.*, 1981, **1**, 36-39 (*17-O-Acetylajmaline, 17-O-Acetylnorajmaline*)
Danieli, B. *et al., Tetrahedron*, 1984, **40**, 5255-5261 (*cmr*)
Johnston, M.D. *et al., J. Het. Chem.*, 1988, **25**, 1803-1807 (*cmr*)
Ruyter, C.M. *et al., Z. Naturforsch., C*, 1988, **43**, 479-484 (*Rauglucine, Acetylrauglucine, Acetylnorrauglucine*)
Alvarez, J.L. *et al., J. Cardiovasc. Pharmacol.*, 1992, **20**, 43-49 (*Prajmalium, pharmacol*)
Köppel, C. *et al., J. Chromatogr.*, 1992, **575**, 87-91 (*Ajmaline, hplc*)
Falkenhagen, H. *et al., Can. J. Chem.*, 1993, **71**, 2201-2203 (*12-Hydroxyajmaline*)
Saeed, S.A. *et al., J. Pharm. Pharmacol.*, 1993, **45**, 715-719 (*Ajmaline, pharmacol*)
Bailey, P.D. *et al., J.C.S. Perkin 1*, 1993, 441-449 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 58; 67
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag*, 1994, 7912 (*synonyms*)
Jokela, R. *et al., Planta Med.*, 1996, **62**, 577-579 (*Isoajmaline, Isosandwicine, pmr, cmr*)
Li, J. *et al., J.A.C.S.*, 1999, **121**, 6998-7010 (*synth*)
Hanhinen, P. *et al., J. Nat. Prod.*, 2001, **64**, 686-687 (*Ajmalimine*)
Wang, T. *et al., Org. Lett.*, 2001, **3**, 345-348 (*synth*)
Itoh, A. *et al., J. Nat. Prod.*, 2005, **68**, 848-852 (*N^b-Methylajmaline, N^b-Methylisoajmaline*)
Lewis, S.E. *et al., Tetrahedron*, 2006, **62**, 8655-8681 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, AFH250; DNB000; AFH280; PNC875

Ajmalinimine A-217

*10-Acetyl-17-*O*-acetylajmaline*



Absolute Configuration

$C_{24}H_{30}N_2O_4$ 410.512

Shown to be an artifact formed from 17-*O*-Acetylajmaline in A-216. Alkaloid from the roots of *Rauwolfia serpentina*. Elongated rods (moist MeOH). Mp 198-199°. $[\alpha]_D^{20}$ +205 (c, 0.3 in $CHCl_3$).

Ac:
Needles. Mp 205-206°.

Siddiqui, S. *et al., Heterocycles*, 1987, **26**, 463 (*isol, uv, ir, pmr, cmr, ms, struct*)
Lounasmaa, M. *et al., Heterocycles*, 2007, **72**, 647-648

Ajmalinine A-218

[73144-99-7]

$C_{22}H_{26}N_2O_3$ 366.459

Struct. unknown. Alkaloid from *Rauwolfia vomitoria* and the roots of *Rauwolfia serpentina* and *Rauwolfia sellowii* (Apocynaceae). Antihypertensive agent. Weak sympatholytic agent. Hexagonal prisms + $1H_2O$ (EtOAc). Mp 180-181°. $[\alpha]_D^{33}$ -97. Conts. OH and OMe but no NMe. Prob conts. a 5-Methoxyindole chromophore. Props. very close to Isorauhimbine in Y-13 isol. from the same sources (Bader *et al*, *Experientia*, 1954). λ_{max} 273 ; 300 (no solvent reported).

Hydrochloride:
Powder (EtOH/Et_2O). Mp 240-245° dec. $[\alpha]_D^{40}$ -44 (c, 1 in H_2O).

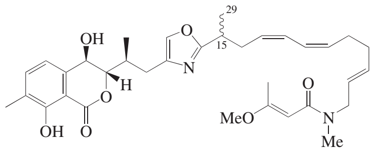
Methiodide:
Rods (EtOH). Mp 233-234° dec.

Picrate:
Yellow powder. Mp 200-205°.

Siddiqui, S. *et al., J. Indian Chem. Soc.*, 1931, **8**, 669-680; 1932, **9**, 539-544; 1935, **12**, 37-47 (*isol*)
Raymond-Hamet, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1953, **237**, 1435-1438 (*uv*)
Bader, F.E. *et al., Experientia*, 1954, **10**, 298 (*bibl*)

Seba, R.A. *et al., CA*, 1955, **49**, 14270e (*isol*)
Bader, F.E. *et al., J.A.C.S.*, 1955, **77**, 3547-3550 (*bibl*)
Malik, A. *et al., Pak. J. Sci. Ind. Res.*, 1979, **22**, 121-123 (*isol*)

Ajudazol B A-219



Relative Configuration

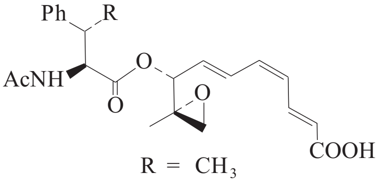
$C_{34}H_{44}N_2O_7$ 592.731
Prod. by *Chondromyces crocatus.* Inhibitor of mitochondrial electron transport. Amorph. solid. $[\alpha]_D^{21}$ +6.1 (c, 1.34 in MeOH). λ_{max} 214 (log ϵ 4.58); 237 (log ϵ 4.54); 306 (sh) ; 319 (log ϵ 3.66) (MeOH).

15,29-Didehydro: ***Ajudazol A***
$C_{34}H_{42}N_2O_7$ 590.715
Prod. by *Chondromyces crocatus.* Inhibitor of mitochondrial electron transport. Amorph. powder. $[\alpha]_D^{21}$ -44.3 (c, 1 in MeOH). λ_{max} 213 (log ϵ 4.67); 235 (log ϵ 4.59); 320 (log ϵ 3.69) (MeOH).

Jansen, R. *et al., Eur. J. Org. Chem.*, 2002, 917-921 (*isol, pmr, cmr*)
Kunze, B. *et al., J. Antibiot.*, 2004, **57**, 151-155 (*activity*)
Buntin, K. *et al., Angew. Chem., Int. Ed.*, 2008, **47**, 4595-4599 (*biosynth*)

AK toxin I A-220

N-*Acetyl-β-methyl-*L*-phenylalanine 7-carboxy-1-(2-methyloxiranyl)-2,4,6-heptatrienyl ester, 9CI*
[85146-09-4]



R = CH_3

$C_{23}H_{27}NO_6$ 413.469
Prod. by *Alternaria alternata* Japanese pear pathotype and *Alternaria kikuchiana*. Phytotoxin. Cryst. (MeOH). Mp 168° dec. $[\alpha]_D^{25}$ +164 (c, 0.128 in MeOH). λ_{max} 285 (ϵ 27600) (MeOH) (Derep).

Nakashima, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 807 (*isol, struct, props*)
Uemura, I. *et al., Tetrahedron*, 2002, **58**, 2351 (*synth*)

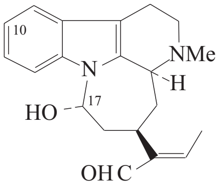
AK toxin II A-221

[85146-10-7]
As AK toxin I, A-220 with
R = H
$C_{22}H_{25}NO_6$ 399.443
Prod. by *Alternaria alternata*. Phytotoxin. Cryst. (MeOH). Mp 163° dec. $[\alpha]_D^{23}$ +125 (c, 0.132 in MeOH). λ_{max} 285 (ϵ 27600) (MeOH) (Derep).

Nakashima, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 807 (*isol, struct, props*)
Ando, K. *et al., Heterocycles*, 1989, **29**, 1023 (*synth*)
Irie, H. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1451 (*synth*)
Uemura, I. *et al., Tetrahedron*, 2002, **58**, 2351 (*synth*)

Akagerine A-222

*α-Ethylidene-1,2,3,3*a*,4,5,6,7-octahydro-7-hydroxy-3-methyl-3,7*a*-diazacyclohepta[*jk*]fluorene-5-acetaldehyde, 9CI*
[56519-07-4]



Absolute configuration

$C_{20}H_{24}N_2O_2$ 324.422
Alkaloid from *Strychnos usambarensis*, *Strychnos gardneri*, *Strychnos jobertiana*, *Strychnos parvifolia*, *Strychnos camptoneura*, *Strychnos spinosa*, *Strychnos nigritana* and *Strychnos decussata*. Convulsant. Platelets (hexane). Sol. MeOH, $CHCl_3$. Mp 188° dec. $[\alpha]_D^{20}$ -16.6 (c, 1 in MeOH). λ_{max} 227 (ϵ 32360); 276 (ϵ 6600); 283 (ϵ 6610); 293 (ϵ 5370) (MeOH) (Berdy).

Me ether: ***17-O-Methylakagerine***
[69241-17-4]
$C_{21}H_{26}N_2O_2$ 338.449
Alkaloid from *Strychnos dale*, *Strychnos decussata* and *Strychnos elaeocarpa* (Loganiaceae). Convulsant. Cryst. (EtOH). Mp 187-189°.

▶ HM1068000

Et ether: ***17-O-Ethylakagerine***
$C_{22}H_{28}N_2O_2$ 352.475
Alkaloid from the root bark of *Strychnos johnsonii* (Loganiaceae). $[\alpha]_D$ -13 (c, 0.6 in MeOH). Poss. an artifact.

10-Hydroxy: ***10-Hydroxyakagerine***
[74765-89-2]
$C_{20}H_{24}N_2O_3$ 340.421
Alkaloid from leaves of *Strychnos spinosa* (Loganiaceae). Cryst. ($CHCl_3$/EtOAc). Mp 149-150°. $[\alpha]_D^{20}$ -4.6 (c, 1 in MeOH).

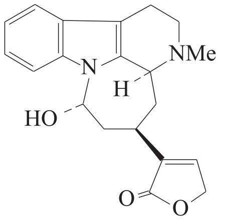
10-Hydroxy, 17-Me ether: ***10-Hydroxy-17-O-methylakagerine***
[73360-05-1]
$C_{21}H_{26}N_2O_3$ 354.448
Alkaloid from *Strychnos decussata* stem bark (Loganiaceae).

▶ HM1060000

Angenot, L. *et al., Tet. Lett.*, 1975, 1357 (*isol, ir, uv, ms, pmr, cryst struct*)
Rolfsen, W. *et al., Planta Med.*, 1978, **34**, 264-273 (*deriv*)
Oguakwa, J. *et al., Gazz. Chim. Ital.*, 1980, **110**, 97-100 (*10-Hydroxyakagerine*)
Rolfsen, W. *et al., J. Nat. Prod.*, 1980, **43**, 97-102 (*10-Hydroxyakagerine, 10-Hydroxy-17-O-methylakagerine*)
Marini-Bettolo, G.B. *et al., J. Nat. Prod.*, 1980, **43**, 717 (*isol*)
Benson, W. *et al., Heterocycles*, 1981, **15**, 935 (*synth*)
Verpoorte, R. *et al., Planta Med.*, 1981, **42**, 32-36 (*isol, uv, pmr*)
Massiot, G. *et al., Phytochemistry*, 1987, **26**, 2839-2846 (*O-Ethylakagerine*)
Danieli, B. *et al., J.O.C.*, 1995, **60**, 2506 (*synth*)
Delaude, C. *et al., Bull. Soc. R. Sci. Liege*, 1997, **66**, 183-286 (*occur, Strychnos*)
Bennasar, M.-L. *et al., J.O.C.*, 1999, **64**, 9605-9612 (*synth*)

Akagerine lactone A-223

[75667-85-5]



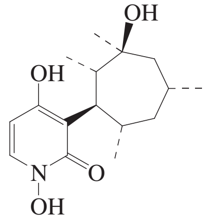
Absolute configuration

$C_{20}H_{22}N_2O_3$ 338.405
Alkaloid from *Strychnos decussata* and from *Strychnos johnsonii* (Loganiaceae). Mp 184-186°.

Et ether: **O-Ethylakagerine lactone**
[113141-70-1]
$C_{22}H_{26}N_2O_3$ 366.459
Alkaloid from root bark of *Strychnos johnsonii* (Loganiaceae). $[\alpha]_D$ -12 (c, 0.4 in $CHCl_3$).

Olaniyi, A.A. *et al., J. Nat. Prod.*, 1980, **43**, 595-597 (*isol, uv, ir, pmr, ms, struct*)
Massiot, G. *et al., Phytochemistry*, 1987, **26**, 2839-2846 (*O-Ethylakagerine lactone*)

Akanthomycin A-224

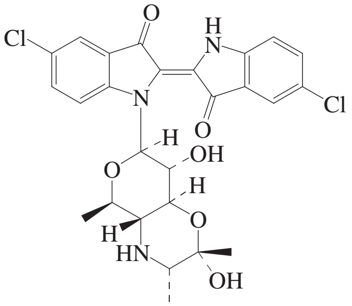


$C_{16}H_{25}NO_4$ 295.378
Isol. from the entomopathogenic fungus *Akanthomyces gracilis.* Antibacterial agent. Cryst. Isol. as a mixt. of two atropisomers.

Wagenaar, M.M. *et al., Org. Lett.*, 2002, **4**, 671-673 (*isol, pmr, cmr*)

Akashin C A-225

[428517-19-5]



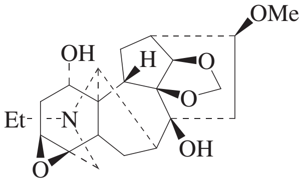
$C_{26}H_{25}Cl_2N_3O_6$ 546.405

N-Glycoside of 6,6′-Dichloroindigotin, D-353. Prod. by *Streptomyces* sp. GW 48/1497. $[\alpha]_D^{25}$ +3100 (c, 0.0058 in MeOH). λ_{max} 241 (log ϵ 4.58); 290 (log ϵ 4.43); 619 (log ϵ 4.2) (MeOH).

Maskey, R.P. *et al., Angew. Chem., Int. Ed.*, 2002, **41**, 597-599 (*isol, pmr, cmr, ms*)
Maskey, R.P. *et al., Nat. Prod. Res.*, 2005, **19**, 137-142 (*struct*)

Akirine A-226

[402821-48-1]



$C_{22}H_{31}NO_6$ 405.49

Alkaloid from *Aconitum kirinense* (Ranunculaceae). Cryst. (Me_2CO). Mp 214-217°.

Nishanov, A.A. *et al., Khim. Prir. Soedin.*, 1992, **28**, 534-537; *Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 466-469 (*isol, pmr, ms, cryst struct*)

Akuammenine A-227

Struct. unknown

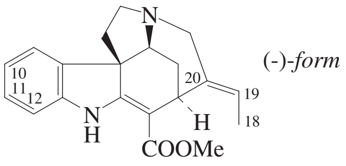
$C_{20}H_{22}N_2O_4$ 354.405

Minor alkaloid from *Picralima klaineana* (Apocynaceae). Scarlet flakes (MeOH)(as picrate). Mp 225° (picrate).

Henry, T.A. *et al., J.C.S.*, 1932, 2759-2768

Akuammicine A-228

Methyl 2,16,19,20-tetradehydrocuran-17-oate, 9CI



$C_{20}H_{22}N_2O_2$ 322.406

(-)-*form* [639-43-0]

Alkaloid from *Catharanthus roseus*, *Picralima nitida*, *Picralima klaineana*, *Amsonia brevifolia*, *Alstonia angustifolia*, *Alstonia scholaris* and other *Alstonia* spp., several *Vinca* spp., *Strychnos angolensis*, *Rauwolfia volkensii*, seeds of *Hunteria congolana*, *Catharanthus microphyllus*, *Cabucala erythrocarpa* leaves, and *Pandaca ochrascens*. Mp 177.5°. $[\alpha]_D^{19}$ -738 ($CHCl_3$). pK_a 7.45. λ_{max} 228 (ϵ 12300); 298 (ϵ 11800); 328 (ϵ 17400) (MeOH) (Berdy).

Hydrochloride: Mp 144° (hydrate) Mp 171° (anhyd.).

Picrate: Mp 169°.

N^b-*Oxide:* ***Akuammicine*** **N^b*-oxide***
[60048-86-4]
$C_{20}H_{22}N_2O_3$ 338.405
Alkaloid from *Alstonia scholaris* root, *Alstonia angustifolia* stem bark, *Rauwolfia* spp. and *Tabernaemontana* spp. (Apocynaceae). Amorph. powder. Mp 200.7-200.8°. $[\alpha]_D^{22}$ -624.5 (c, 0.55 in $CHCl_3$).

N^b-*Me:* ***Akuammicine*** **N^b*-methosalt***
[100680-12-4]
$C_{21}H_{25}N_2O_2^{\oplus}$ 337.441
Alkaloid from *Alstonia scholaris*, root and stem bark of *Hunteria eburnea* and leaves of *Vinca minor* (Apocynaceae). Mp 270° dec. (as chloride). $[\alpha]_D^{20}$ -120 (c, 0.1 in EtOH) (chloride). CAS no. refers to chloride.

19,20S-Dihydro: ***19,20-Dihydroakuammicine***
[2912-08-5]
$C_{20}H_{24}N_2O_2$ 324.422
Minor alkaloid from leaves of *Pleiocarpa pycnantha* var. *tubicina* and *Rauwolfia caffra* (Apocynaceae). Mp 169-171°. $[\alpha]_D^{27}$ -636.6 (c, 0.74 in MeOH).

19α,20α-Epoxide: ***19,20-Epoxyakuammicine***
[173658-92-9]
$C_{20}H_{22}N_2O_3$ 338.405
Alkaloid from leaves of *Rauwolfia sellowii* (Apocynaceae). No phys. props. reported.

10-Hydroxy: ***Sewarine***. *10-Hydroxyakuammicine*
[27160-72-1]
$C_{20}H_{22}N_2O_3$ 338.405
Alkaloid from leaves of *Rauwolfia stricta* and leaves and roots of *Rhazya stricta* (Apocynaceae). Shows cytotoxic activity. Cryst. or off-white powder. Mp 245° dec. $[\alpha]_D^{20}$ -720 (c, 0.1 in EtOH). λ_{max} 220 (ϵ 10800); 311 (ϵ 14400); 340 (ϵ 11900) (MeOH).

10-Hydroxy; hydrochloride: Mp 210° dec. $[\alpha]_D^{32}$ -724 (EtOH).

12-Hydroxy: ***Vinervine***. *12-Hydroxyakuammicine*
[1963-86-6]
$C_{20}H_{22}N_2O_3$ 338.405
Originally considered to be 11-Hydroxyakuammicine. Alkaloid from *Vinca erecta* upper parts, also obt. from cell suspension cultures of *Stemmadenia tomentosa* (Apocynaceae). Mp 154-155° dec. λ_{max} 234 (log ϵ 4.22); 290 (log ϵ 3.86); 336 (log ϵ 4.22) (EtOH).

19,20-Dihydro, 19-hydroxy: see Echitamidine, E-30

19,20-Dihydro, hydroxy: ***Hydroxy-19,20-dihydroakuammicine***
[59981-20-3]
$C_{20}H_{24}N_2O_3$ 340.421
Minor alkaloid from *Alstonia scholaris* root bark (Apocynaceae). Amorph. powder. Appears to be distinct from the 18- or 19-hydroxy compd. above. Could be identical with Echitamidine, E-30 or a stereo- or regioisomer of it.

19,20-Dihydro, 18- or 19-hydroxy: ***18(19)-Hydroxy-19,20-dihydroakuammicine***
$C_{20}H_{24}N_2O_3$ 340.421
Minor alkaloid from *Alstonia scholaris* root bark (Apocynaceae). Amorph. powder. Not compared with Echitamidine, could be identical or a stereo- or regioisomer of it.

11-Methoxy: ***11-Methoxyakuammicine***
[54484-54-7]
$C_{21}H_{24}N_2O_3$ 352.432
Minor alkaloid from *Alstonia muelleriana* bark, *Alstonia lanceolifera* stem bark, *Alstonia odontophora* and other *Alstonia* spp. (Apocynaceae). $[\alpha]_D$ -505 (EtOAc). Originally considered to be identical with Vinervinine, but when the struct. of Vinervinine was revised to 12-methoxyakuammicine it was reexamined and found to be different. λ_{max} 232 (ϵ 11500); 305 (ϵ 5620); 324 (ϵ 6525) (MeOH).

11-Methoxy, N^b*-oxide:* ***11-Methoxyakuammicine*** **N^b*-oxide***
[94444-35-6]
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from leaves of *Alstonia macrophylla* (Apocynaceae). Solid. $[\alpha]_D^{25}$ -419.1 (c, 2.65 in MeOH).

11-Methoxy, 19,20α-epoxide: ***Alstolagumine***. *11-Methoxy-19,20α-epoxyakuammicine*
[154849-51-1]
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from leaves of *Alstonia macrophylla* (Apocyanaceae). Solid. $[\alpha]_D^{22}$ -73.4 (c, 1.30 in MeOH).

12-Methoxy: ***Vinervinine***. *12-Methoxyakuammicine*
[17366-53-9]
$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from the epigeal parts of *Vinca major* and *Vinca erecta* (Apocynaceae). Mp 190-191°. $[\alpha]_D^{20}$ -564 (c, 1.877 in $CHCl_3$).

12-Methoxy, N^b*-Me:* ***12-Methoxy-*****N^b*-methylakuammicine***
[123064-76-6]
$C_{22}H_{27}N_2O_3^{\oplus}$ 367.467
Quaternary alkaloid from the root bark of *Alstonia congensis* (Apocynaceae). $[\alpha]_D$ +70 (c, 0.15 in $CHCl_3$) (as 3-pyridinecarboxylate). λ_{max} 225 ; 282 ; 289 ; 333 (MeOH) (3-pyridinecarboxylate).

12-Methoxy, 19α,20α-epoxide: ***12-Methoxy-19α,20α-epoxyakuammicine***
[104696-13-1]
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from the leaves of *Amsonia lenormandii* var. *lenormandii* (Apocynaceae). Cryst. (Et_2O). Mp 188°. $[\alpha]_D$ -590 (c, 1 in $CHCl_3$).

19,20α-Dihydro, 19-oxo, 20-hydroxy: Lagumicine
$C_{20}H_{22}N_2O_4$ 354.405
Alkaloid from the leaves of *Alstonia angustifolia* var. *latifolia*. Light yellow oil. $[\alpha]_D$ -552 (c, 0.07 in $CHCl_3$). λ_{max} 234 (log ϵ 3.79); 294 (log ϵ 3.71); 328 (log ϵ 3.85) (EtOH).

Δ^{18}-Isomer: ***Angustimicine***
[54086-20-3]
$C_{20}H_{22}N_2O_2$ 322.406

Alkaloid from *Amsonia angustifolia* (Apocynaceae). Struct. appears dubious. The obvious intercorrelation with Akuammicine has not been carried out.

(±)-form

Pseudakuammicine. Pseudoakuammicine

[7344-80-1]

Alkaloid from seeds of *Picralima nitida* (Apocynaceae). Mp 187.5°.

Hydrochloride:

Minute needles (EtOH or H_2O). Mp 216°.

Henry, T.A. *et al., J.C.S.*, 1927, 1950-1959; 1932, 2759-2768 (*isol*)

Aghoramurthy, K. *et al., Tetrahedron*, 1957, **1**, 172 (*isol, struct*)

Lévy, J. *et al., Bull. Soc. Chim. Fr.*, 1960, 979-981 (*Akuammicine*)

Edwards, P.N. *et al., J.C.S.*, 1961, 152-165 (*abs config*)

Bartlett, M.F. *et al., J.O.C.*, 1963, **28**, 1445-1449 (*isol, synth, methosalt*)

Budzikiewicz, H. *et al., Tetrahedron*, 1963, **19**, 1265-1276 (*ms*)

Kump, W.G. *et al., Helv. Chim. Acta*, 1964, **47**, 1497-1503 (*19,20-Dihydroakuammicine*)

Kuchenkova, M.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1965, 2152; *CA*, **64**, 11269c (*Vinervine, isol*)

Yuldashev, P.Kh. *et al., Khim. Prir. Soedin.*, 1965, **1**, 34-42; 1967, **3**, 310-315; 1974, **10**, 260-261; 1983, **19**, 210-212; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 25-30; 1967, **3**, 263-266; 1974, **10**, 276-277; 1983, **19**, 199-201 (*Vinervine, Vinervinine, isol, cmr, struct, bibl*)

Ahmad, Y. *et al., J. Pharm. Sci.*, 1971, **60**, 1581-1583 (*Sewarine, isol, uv, ms*)

Karle, J.M. *et al., Chem. Comm.*, 1972, 416-417 (*Sewarine, cryst struct*)

Burke, D.E. *et al., Phytochemistry*, 1973, **12**, 1467-1474 (*11-Methoxyakuammicine*)

Böjthe-Korvath, K. *et al., CA*, 1974, **81**, 136347 (*Angustimicine*)

Kutney, J.P. *et al., Heterocycles*, 1975, **3**, 197-204 (*synth*)

Burke, D.E. *et al., J.O.C.*, 1975, **40**, 1367-1368 (*11-Methoxyakuammicine*)

Boonchuay, W. *et al., Phytochemistry*, 1976, **15**, 821 (*Alstonia scholaris alkaloids*)

Akinloye, B.A. *et al., Phytochemistry*, 1980, **19**, 307-311 (*Sewarine, isol, uv, ms, ir*)

Mukopadhyay, S. *et al., J. Nat. Prod.*, 1981, **44**, 696-700 (*Sewarine, isol, pharmacol*)

Ravao, T. *et al., Phytochemistry*, 1982, **21**, 2160-2161 (*11-Methoxyakuammicine, Angustimicine*)

Stöckigt, J. *et al., Z. Naturforsch., C*, 1982, **37**, 857-860 (*Vinervine, isol*)

Legseir, B. *et al., Phytochemistry*, 1986, **25**, 1735-1738 (*12-Methoxy-19,20-epoxyakuammicine*)

Caron, C. *et al., Phytochemistry*, 1989, **28**, 1241-1244 (*12-Methoxy-N^b-methylakuammicine*)

Proksa, B. *et al., Planta Med.*, 1989, **55**, 188-190 (*Akuammicine N-methosalt*)

Hu, W.-L. *et al., Planta Med.*, 1989, **55**, 463-466 (*Akuammicine N-oxide*)

Amat, M. *et al., J.O.C.*, 1990, **55**, 6299-6312 (*19,20-Dihydroakuammicine, synth*)

Abe, F. *et al., Phytochemistry*, 1994, **35**, 249-252; 253-257 (*11-Methoxyakuammicine N^b-oxide, 11-Methoxy-19,20α-epoxyakuammicine*)

Solé, D. *et al., J.O.C.*, 1996, **61**, 4194-4195 (*synth*)

Batista, C.V.F. *et al., Phytochemistry*, 1996, **41**, 969-973 (*epoxide*)

Bonjoch, J. *et al., J.A.C.S.*, 1997, **119**, 7230-7240 (*synth*)

Ito, M. *et al., J.A.C.S.*, 2001, **123**, 8003-8010 (*synth*)

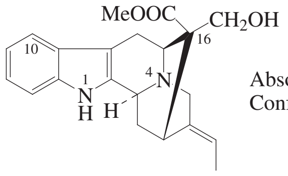
Salim, A.A. *et al., J. Nat. Prod.*, 2004, **67**, 1591-1594 (*oxide*)

Kam, T.-S. *et al., Phytochemistry*, 2004, **65**, 603-608 (*Lagumicine*)

Akuammidine A-229

Methyl 17-hydroxysarpagan-16-carboxylate, 9CI†. Rhazine

[639-36-1]



Absolute Configuration

$C_{21}H_{24}N_2O_3$ 352.432

Pmr and cmr spectral data revised in 1996. Alkaloid from *Picralima nitida*, *Amsonia brevifolia*, *Rauwolfia vomitoria*, *Picralima nitida*, *Rhazya stricta*, *Strychnos angolensis* and *Strychnos potatorum*. Mp 234-236° Mp 265°.

Picrate:

Yellow spheroids (EtOH). Mp 215°.

N^4-*Me:* ***Macusine C***

[6801-17-8]

$C_{22}H_{27}N_2O_3^{\oplus}$ 367.467

Quaternary alkaloid from the bark of *Strychnos toxifera* (Loganiaceae). Cryst. (EtOH/Et_2O) (as chloride). Mp 264-265° (260-261°) dec. (chloride). $[\alpha]_D^{24}$ -60.8 (c, 2.13 in H_2O) (chloride).

O-*Ac:*

Prisms ($CHCl_3$/EtOH). Mp 272°.

Z-Isomer: ***(Z)-Akuammidine***

[113973-31-2]

$C_{21}H_{24}N_2O_3$ 352.432

Alkaloid from roots of *Gelsemium elegans*. Needles (Me_2CO). Mp 240-242°. $[\alpha]_{Hg}^{16}$ +9 (c, 0.16 in MeOH).

10-Methoxy, N^1-*Me:* **N^a*-Methyl-10-methoxyakuammidine***

[56440-63-2]

$C_{23}H_{28}N_2O_4$ 396.485

Alkaloid from the aerial parts of *Alstonia lanceolifera* and *Alstonia boulindaensis* (Apocynaceae). Mp 234-236°. $[\alpha]_D$ +52 (c, 1 in $CHCl_3$).

16-Epimer: see Polyneuridine, P-562

Chatterjee, A. *et al., Chem. Ind. (London)*, 1961, 1034-1035 (*isol, uv, ir*)

Chatterjee, A. *et al., J. Sci. Ind. Res., Sect. B*, 1962, **21**, 147 (*pmr*)

Silvers, S. *et al., Tet. Lett.*, 1962, 339-343 (*cryst struct*)

Ohashi, M. *et al., Tetrahedron*, 1963, **19**, 2241-2246 (*ms*)

Battersby, A.R. *et al., J.C.S.*, 1964, 4419-4427 (*Macusine C*)

Bláha, K. *et al., Coll. Czech. Chem. Comm.*, 1974, **39**, 3168-3176 (*uv, cd, ord*)

Lewin, G. *et al., Phytochemistry*, 1975, **14**, 2067-2071 (*N^a-Methyl-10-methoxyakuammidine*)

Jewers, K. *et al., Planta Med.*, 1980, **38**, 359-362 (*cmr*)

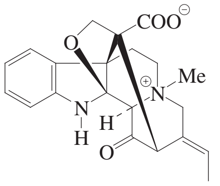
Ponglux, D. *et al., Tetrahedron*, 1988, **44**, 5075-5094 (*Z-isomer*)

Lin, L. *et al., Phytochem. Anal.*, 1990, **1**, 26 (*pmr, cmr, Z-isomer*)

Jokela, R. *et al., Heterocycles*, 1996, **43**, 1015-1020 (*pmr, cmr*)

Akuammiginone A-230

[761445-62-9]



Relative Configuration

$C_{21}H_{22}N_2O_4$ 366.416

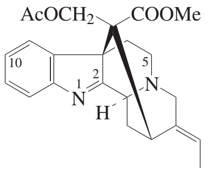
Alkaloid from the bark of *Alstonia scholaris*. Amorph. light yellow powder. $[\alpha]_D^{25}$ +23.4 (c, 0.5 in MeOH). Zwitterionic. λ_{max} 221 (log ϵ 3.7); 232 (log ϵ 3.69); 286 (log ϵ 3.36) (MeOH).

Salim, A.A. *et al., J. Nat. Prod.*, 2004, **67**, 1591-1594 (*isol, pmr, cmr*)

Akuammiline A-231

Methyl 17-(acetyloxy)akuammilan-16-carboxylate, 10CI. Methyl 16-[(acetyloxy)methyl]akuammilan-17-oate, 9CI

[1897-26-3]



Absolute Stereochemistry

$C_{23}H_{26}N_2O_4$ 394.469

Alkaloid from *Picralima nitida, Conopharyngia durissima, Vinca minor, Rauwolfia oreogiton* and *Rauwolfia vomitoria* (Apocynaceae). Cryst. (Et_2O). Mp 157-161°. $[\alpha]_D^{24}$ +83 (c, 0.5 in $CHCl_3$).

Hydrochloride:

Cryst. + $1H_2O$ (H_2O or EtOH). Mp 196°. $[\alpha]_D^{20}$ -29.6 (c, 3.84 in H_2O).

Methiodide:

Needles (H_2O). Mp 233°. $[\alpha]_D^{20}$ -83 (c, 1.36 in EtOH).

N^4-*Oxide:* ***Akuammiline*** **N^4*-oxide***

$C_{23}H_{26}N_2O_5$ 410.469

Alkaloid from *Kopsia griffithii*. $[\alpha]_D$ -144 (c, 0.13 in $CHCl_3$). λ_{max} 222 (log ϵ 4.35); 270 (log ϵ 3.77) (EtOH).

O-*De-Ac:* ***Rhazimol***. *Deacetylakuammiline. Ercinaminine*

[1897-30-9]

$C_{21}H_{24}N_2O_3$ 352.432

Alkaloid from *Vinca minor, Picralima nitida, Rauwolfia vomitoria, Rauwolfia oreogiton* and *Rhazya stricta* (Apocynaceae). Pale yellow amorph. powder. $[\alpha]_D^{21}$ +19.7 (MeOH).

O-*De-Ac,* O-*(3,4,5-trimethoxybenzoyl):* ***Alstolenine***

[85769-33-1]

$C_{31}H_{34}N_2O_7$ 546.619
Minor alkaloid from the leaves of *Alstonia venenata*. Amorph. $[\alpha]_D$ -70.9 (EtOH).

1,2β-Dihydro: ***1,2β-Dihydroakuammiline***
[77485-26-8]
$C_{23}H_{28}N_2O_4$ 396.485
Alkaloid from the leaves of *Rauwolfia oreogiton* (Apocynaceae). Off-white amorph. powder. $[\alpha]_D^{21}$ -9.4 (MeOH).

1,2β-Dihydro, O*-de-Ac:* ***Deacetyl-1,2β-dihydroakuammiline***
[77485-27-9]
$C_{21}H_{26}N_2O_3$ 354.448
Alkaloid from the leaves of *Rauwolfia oreogiton* (Apocynaceae). Mp 228-230°. $[\alpha]_D^{21}$ +99 (MeOH).

5-Oxo, 1,2ξ-dihydro, O*-de-Ac:* ***Deacetyl-1,2-dihydro-5-oxoakuammiline***
[870995-65-6]
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from the leaves of *Alstonia scholaris*. Powder. Mp 290-292°. $[\alpha]_D^{13}$ -147.5 (c, 0.35 in $CHCl_3$).

10-Hydroxy, O*-de-Ac:* ***Ercinamine***. *10-Hydroxydeacetylakuammiline*
[85783-98-8]
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from *Catharanthus roseus* and *Vinca erecta*. Mp 238-240°. $[\alpha]_D$ +53.

10-Methoxy: ***Raufloricine***
[38734-62-2]
$C_{24}H_{28}N_2O_5$ 424.496
Alkaloid from *Vinca minor* and from the root bark of *Rauwolfia confertiflora* (Apocynaceae). Cryst. (Me_2CO/hexane or EtOAc). Mp 190-193°. $[\alpha]_D^{20}$ +129 (c, 1.5 in $CHCl_3$).

10-Methoxy, O*-de-Ac:* ***Nervobscurine***. *10-Methoxydeacetylakuammiline*
[38734-63-3]
$C_{22}H_{26}N_2O_4$ 382.458
Alkaloid from *Vinca minor*. Amorph. $[\alpha]_D^{25}$ +83 (c, 0.72 in EtOH).

5α,10-Dimethoxy, O*-de-Ac,* O*-benzoyl:* ***Deacetyl-O-benzoyl-5,10-dimethoxyakuammiline***
$C_{30}H_{32}N_2O_6$ 516.593
Alkaloid from *Alstonia villosa*. Solid. $[\alpha]_D^{20}$ -169.7 (c, 0.38 in MeOH).

5α,10-Dimethoxy, O*-de-Ac,* O*-(3,4,5-trimethoxybenzoyl):* ***5,10-Dimethoxyalstolenine***
$C_{33}H_{38}N_2O_9$ 606.671
Alkaloid from *Alstonia villosa*. Prisms. Mp 190-192°. $[\alpha]_D^{25}$ -213 (c, 0.82 in $CHCl_3$). λ_{max} 218 (log ε 4.71); 279 (log ε 4.22); 300 (sh) (log ε 4.13) (MeOH).

5β,11-Dimethoxy, O*-de-Ac:* ***Deacetyl-5β,11-dimethoxyakuammiline***
$C_{23}H_{28}N_2O_5$ 412.485
Alkaloid from the roots of *Rauwolfia yunnanensis*. Amorph. yellow solid. $[\alpha]_D^{24}$ -124 (c, 0.46 in Py). λ_{max} 208 (log ε 4.24); 224 (log ε 4.2); 230 (log ε 4.21); 289 (log ε 3.53) (MeOH).

5β-Hydroxymethyl: ***5-Hydroxymethylakuammiline***
[77485-24-6]
$C_{24}H_{28}N_2O_5$ 424.496
Alkaloid from the leaves of *Rauwolfia oreogiton* (Apocynaceae). Off-white amorph. powder. $[\alpha]_D^{21}$ -141 (MeOH).

16-Epimer: ***16-Epiakuammiline***
[958247-21-7]
$C_{23}H_{26}N_2O_4$ 394.469
Alkaloid from *Kopsia singapurensis*. Oil. $[\alpha]_D^{25}$ +116 (c, 0.23 in $CHCl_3$). λ_{max} 210 (log ε 3.99); 220 (log ε 4.05); 265 (log ε 3.35) (EtOH).

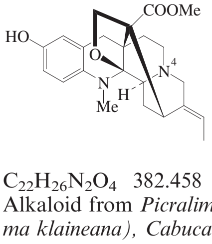
16-Epimer, O*-de-Ac:* ***16-Epideacetylakuammiline***
$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from the stem bark of *Kopsia deverrei*. $[\alpha]_D^{20}$ +232 (c, 0.53 in $CHCl_3$). λ_{max} 220 (log ε 4.22); 265 (log ε 3.18) (EtOH).

16-Epimer, O*-de-Ac,* N^4*-oxide:* ***16-Epideacetylakuammiline*** N^4***-oxide***
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from *Kopsia griffithii*. $[\alpha]_D$ -66 (c, 0.15 in $CHCl_3$). λ_{max} 222 (log ε 4.12); 272 (log ε 3.57) (EtOH).

Henry, T.A. *et al., J.C.S.*, 1932, 2759 (*isol*)
Dugan, J.J. *et al., Helv. Chim. Acta*, 1969, **52**, 701 (*isol, uv, ir, pmr, ms*)
Savaşkan, S. *et al., Helv. Chim. Acta*, 1972, **55**, 2861 (*Akuammiline, Raufloricine, Nervobscurine*)
De Maindreville, M.D. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1975, **280**, 131 (*config*)
Akinloye, B.A. *et al., Phytochemistry*, 1980, **19**, 2741 (*Dihydroakuammiline, Rhazimol, Deacetyldihydroakuammiline*)
Majumder, P. *et al., Phytochemistry*, 1982, **21**, 2389 (*Alstolenine*)
Gueritte, F. *et al., J. Nat. Prod.*, 1983, **46**, 144 (*Ercinamine*)
Yagudaev, M.R. *et al., Khim. Prir. Soedin.*, 1983, **19**, 483; *Chem. Nat. Compd. (Engl. Transl.)*, 1983, **19**, 454 (*Ercinamine, Ercinaminine*)
Kan, C. *et al., Nat. Prod. Lett.*, 1995, **7**, 275 (*16-Epideacetylakuammiline*)
Abe, F. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1235-1238 (*5,10-Dimethoxydeacetylakuammilines*)
Kam, T.-S. *et al., Phytochemistry*, 1999, **50**, 75-79 (*N^4-oxides*)
Zhou, H.-U. *et al., Helv. Chim. Acta*, 2005, **88**, 2508-2512 (*Deacetydihydrooxoakuammiline*)
Hu, X.-J. *et al., Helv. Chim. Acta*, 2006, **89**, 1344-1350 (*Deacetyl-5,11-dimethoxyakuammiline*)
Subramaniam, G. *et al., J. Nat. Prod.*, 2007, **70**, 1783-1789 (*16-Epiakuammiline*)

Akuammine A-232

Vincamajoridine
[3512-87-6]



Absolute configuration

$C_{22}H_{26}N_2O_4$ 382.458
Alkaloid from *Picralima nitida (Picralima klaineana), Cabucala erythrocarpa* and *Vinca herbacea* (Apocynaceae). Needles (EtOH). Mp 255° Mp 278-280° (295°). $[\alpha]_D^{20}$ -73.4 (c, 0.87 in $CHCl_3$).

Hydrochloride:
Cryst. + $1H_2O$. Mp 227°. $[\alpha]_D^{22}$ -26.6 (c, 0.88 in H_2O).

Picrate:
Yellow needles (EtOH). Mp 199°.

N^4*-Oxide:* ***Akuammine N-oxide***
$C_{22}H_{26}N_2O_5$ 398.458
Alkaloid from *Vinca major*. Cryst. (EtOH). Mp 178-180°. λ_{max} 243 (log ε 2.91); 312 (log ε 3.21) (EtOH).

Ac:
Prisms (EtOH). Mp 226°. $[\alpha]_D^{20}$ -52.1 (c, 0.64 in EtOH).

Me ether: **O*-Methylakuammine***
[36101-52-7]
$C_{23}H_{28}N_2O_4$ 396.485
Alkaloid from *Rauwolfia oreogiton, Vinca erecta* and *Cabucala fasciculata* (Apocynaceae). Needles (Me_2CO). Mp 242-243°.

10-Deoxy: ***Pseudoakuammigine***. *ψ-Akuammigine*
[2447-70-3]
$C_{22}H_{26}N_2O_3$ 366.459
Alkaloid from *Alstonia scholaris, Picralima klaineana* and *Picralima nitida* (Apocynaceae). Prisms (EtOH aq.), plates (C_6H_6/cyclohexane). Mp 165° (158°). $[\alpha]_D^{20}$ -53.8 (c, 3.42 in EtOH).

10-Deoxy; hydrochloride:
Prisms (H_2O). Mp 183° (solvate) Mp 218° (anhyd.). $[\alpha]_D^{20}$ -15.4 (c, 1.065 in EtOH).

10-Deoxy, picrate:
Yellow needles (Me_2CO). Mp 223°.

10-Deoxy, N^4*-oxide:* ***Pseudoakuammigine N-oxide***
[125205-49-4]
$C_{22}H_{26}N_2O_4$ 382.458
Alkaloid from the stem bark of *Alstonia angustifolia* (Apocynaceae). Mp 204.3-204.4°. $[\alpha]_D^{22}$ -11.5 (c, 0.17 in $CHCl_3$).

*10-Deoxy, 17*S*-hydroxy:* ***17-Hydroxy-ψ-akuammigine***. *10-Deoxy-17-hydroxyakuammine. 17-Hydroxypseudoakuammigine*
[79839-00-2]
$C_{22}H_{26}N_2O_4$ 382.458
Alkaloid from *Hunteria congolana* (Apocynaceae). Mp 131°. $[\alpha]_D$ -8.6 (c, 0.5 in $CHCl_3$).

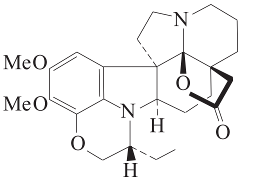
*10-Deoxy, 17*S*-methoxy:* ***17-Methoxy-ψ-akuammigine***
[84959-48-8]
$C_{23}H_{28}N_2O_4$ 396.485
Alkaloid from *Hunteria congolana* (Apocynaceae). Cryst. (Et_2O). $[\alpha]_D$ -8 (c, 0.5 in Et_2O).

Henry, T.A. *et al., J.C.S.*, 1927, 1950 (*isol*)
Joule, J.A. *et al., J.C.S.*, 1962, 312 (*struct, derivs*)
Olivier, L. *et al., Bull. Soc. Chim. Fr.*, 1965, 868 (*struct, abs config*)
Rakhimov, D.A. *et al., Khim. Prir. Soedin.*, 1971, **7**, 677; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 663 (*isol, uv, ir, pmr, ms, struct, O-Methylakuammine*)
Morita, Y. *et al., Helv. Chim. Acta*, 1977, **60**, 1419 (*isol, Pseudoakuammigine*)
Banerji, A. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 390 (*isol, uv, ir, pmr, ms, Pseudoakuammigine*)
Akinloye, B.A. *et al., Phytochemistry*, 1980, **19**, 2741 (*isol, O-Methylakuammine*)
Vercauteren, J. *et al., Tet. Lett.*, 1981, **22**, 2871 (*17-Hydroxy-ψ-akuammigine, Pseudoakuammigine*)

Vercauteren, J. *et al., Bull. Soc. Chim. Fr., Part II*, 1982, 291 (*derivs*)
Zhukovich, E.N. *et al., Khim. Prir. Soedin.*, 1989, **25**, 434-435; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 378 (*N-oxide*)
Hu, W.-L. *et al., Planta Med.*, 1989, **55**, 463 (*Pseudoakuammigine N-oxide*)

Alalakine A-233

22-Ethyl-19-hydroxy-15,16-dimethoxy-4,5-secoobscurinervan-21-oic acid γ-lactone, 9CI
[68346-07-6]

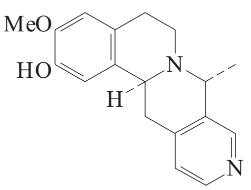


Relative configuration

$C_{25}H_{32}N_2O_5$ 440.538
Alkaloid from *Aspidosperma album* (Apocynaceae). Cryst. (Me_2CO/hexane). Mp 195°. $[\alpha]_D$ -38 ($CHCl_3$).

Urrea, M. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1978, **287**, 63 (*ir, uv, ms, pmr, struct*)

Alamaridine A-234



$C_{18}H_{20}N_2O_2$ 296.368

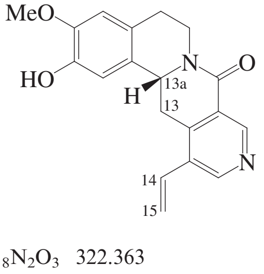
Natural-*form*
Alkaloid from the seeds of *Alangium lamarckii* (Alangiaceae). Light-yellow needles (MeOH). Mp 196°. Opt. rotn. not determined due to paucity of material. λ_{max} 226 (sh) (log ε 3.85); 258 (log ε 3.35); 286 (log ε 3.31) (EtOH).

(±)-*form* [107588-71-6]
Synthetic. Pale yellow granules (MeOH). Mp 242-244°.

Bhattacharjya, A. *et al., Tetrahedron*, 1988, **44**, 3477-3488 (*isol, uv, ir, pmr, ms, synth, struct*)
Reimann, E. *et al., Monatsh. Chem.*, 1994, **125**, 1397-1406 (*synth*)

Alangimaridine A-235

*12-Ethenyl-5,6,13,13*a*-tetrahydro-2-hydroxy-3-methoxy-8*H*-isoquino[2,1-*b*][2,7]naphthyridin-8-one, 9CI*
[77173-59-2]



$C_{19}H_{18}N_2O_3$ 322.363

(*R*)-*form* [178121-46-5]
Alkaloid from the seeds of *Alangium lamarckii* (Alangiaceae). Cryst. (MeOH/ $CHCl_3$). Mp 278°. $[\alpha]_D$ +429 (c, 0.35 in $CHCl_3$).
Ac:
Cryst. (MeOH). Mp 232°.
*13,13*a*-Didehydro:* ***Alangimarine***
[77156-16-2]
$C_{19}H_{16}N_2O_3$ 320.347
Alkaloid from the seeds of *Alangium lamarckii* (Alangiaceae). Mp 247°. Achiral.
*13,13*a*-Didehydro, Ac:* Mp 202°.
*13,13*a*-Didehydro,* O*-de-Me,* O^2*-Me:* ***Isoalangimarine***
[96422-49-0]
$C_{19}H_{16}N_2O_3$ 320.347
Alkaloid from the seeds of *Alangium lamarckii* (Alangiaceae). Yellow needles ($CHCl_3$/MeOH). Mp 249°.
14-Oxo, 13,13a-didehydro, 14,15-dihydro: ***Alangimarinone***
[96422-50-3]
$C_{19}H_{16}N_2O_4$ 336.346
Alkaloid from the seeds of *Alangium lamarckii* (Alangiaceae). Yellow needles. Mp 282°.
14ξ-Hydroxy, 14,15-dihydro: ***Dihydroalamarine***
[97168-61-1]
$C_{19}H_{20}N_2O_4$ 340.378
Alkaloid from the seeds of *Alangium lamarckii* (Alangiaceae). Pale-yellow needles ($CHCl_3$/MeOH). Mp 252-253°. $[\alpha]_D$ +347 (c, 0.35 in Py).
14ξ-Hydroxy, 14,15-dihydro, O*-de-Me,* O^2*-Me:* ***Dihydroisoalamarine***
[96422-51-4]
$C_{19}H_{20}N_2O_4$ 340.378
Alkaloid from the seeds of *Alangium lamarckii* (Alangiaceae). Yellow needles ($CHCl_3$/MeOH). Mp 268-270°. $[\alpha]_D$ +140 (c, 0.07 in Py).
14ξ-Hydroxy, 13,13a-didehydro, 14,15-dihydro: ***Alamarine***
[77156-18-4]
$C_{19}H_{18}N_2O_4$ 338.362
Alkaloid from the seeds of *Alangium lamarckii* (Alangiaceae). Yellow needles ($CHCl_3$/MeOH). Mp 288°. $[\alpha]_D$ 0 ($CHCl_3$).
*14ξ-Hydroxy, 13,13*a*-didehydro, 14,15-dihydro,* O*-de-Me,* O^2*-Me:* ***Isoalamarine***
[77156-20-8]
$C_{19}H_{18}N_2O_4$ 338.362
Alkaloid from the seeds of *Alangium lamarckii* (Alangiaceae). Yellow needles (MeOH/$CHCl_3$). Mp 301-303°.

(±)-*form*
Synthetic. Cryst. (MeOH/$CHCl_3$). Mp 242-245°.

Pakrashi, S.C. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 19-28 (*Alangimarine, Alangimaridine, Isoalangimarine, Alangimarinone, Alamarine, Dihydroalamarine, Dihydroisoalamarine, Isoalamarine,isol, uv, ir, pmr, ms, cd, struct*)
Jahangir, *et al., Can. J. Chem.*, 1987, **65**, 2362-2368 (*Alangimarine, Alangimaridine, synth, ir, pmr, cmr, ms*)
Chowdhury, U.S. *et al., Tetrahedron*, 1990, **46**, 7893-7900 (*Isoalamarine, synth*)
Itoh, A. *et al., J. Nat. Prod.*, 1996, **59**, 535-538 (*Alangimaridine, Alangimarine, synth, cd, abs config*)
Reimann, E. *et al., Monatsh. Chem.*, 2005, **136**, 193-209 (*Alangimarine, synth*)

Alangine A A-236

[6793-39-1]

$C_{15}H_{23}NO_2$ 249.352
Struct. unknown. Alkaloid from *Alangium lamarckii* (Alangiaceae). Cryst. (Et_2O/hexane). Mp 85°. $[\alpha]_D$ -41.3 (c, 0.9 in $CHCl_3$). Was assigned the struct. 3-(4-methoxyphenyl)-2-(1-piperidyl)-1-propanol, but synthetic material differed from the alkaloid.
Hydrochloride:
Cryst. (EtOH/Et_2O). Mp 250°.
Methiodide:
Cryst. (Me_2CO/Et_2O). Mp 184°.
Picrate:
Cryst. (EtOH). Mp 138°.

Bhakuni, D.S. *et al., J. Sci. Ind. Res., Sect. B*, 1960, **19**, 8-10; *CA*, **54**, 21168h
Kapil, R.S. *et al., J. Sci. Ind. Res.*, 1961, **20**, 136; *CA*, **55**, 18792g

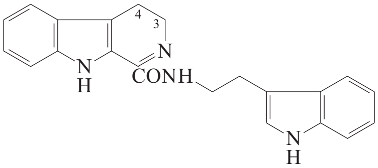
Alanginine A-237

Struct. unknown. Alkaloid from the root bark of *Alangium lamarckii* (Alangiaceae). Cream-coloured amorph. solid. Mp 245-247°.

Singh, M.P. *et al., Proc. Natl. Acad. Sci., India, Sect. A*, 1948, **17**, 1-6; *CA*, **45**, 10489h

Alangiobussine A-238

[171090-88-3]

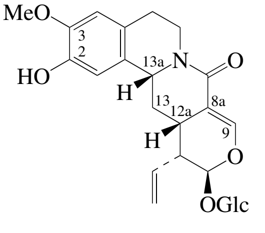


$C_{22}H_{20}N_4O$ 356.426
Alkaloid from leaves of *Alangium bussyanum*. Cryst. (MeOH). Mp 152-154°. λ_{max} 220 (log ε 4.93); 250 (sh) (log ε 4.49); 290 (log ε 4.18); 334 (log ε 4.31) (MeOH).
3,4-Didehydro: ***Alangiobussinine***
[171090-89-4]
$C_{22}H_{18}N_4O$ 354.41
Trace alkaloid from leaves of *Alangium bussyanum* (Alangiaceae). Cryst. (MeOH). Mp 188-190°.

Diallo, A.O. *et al., Phytochemistry*, 1995, **40**, 975-977 (*isol, uv, pmr, cmr, ms*)

Alangiside A-239

[34482-51-4]



$C_{25}H_{31}NO_{10}$ 505.521
Alkaloid from the roots, leaves and fruit of *Alangium lamarckii* (best source unripe fruit) (Alangiaceae). Amorph. powder + 2.5 H_2O. Mp 187° dec. (shrinks at 164°). $[\alpha]_D^{26}$ -105 (c, 1.0 in MeOH).

Tetra-Ac:
Amorph. powder. $[\alpha]_D^{21}$ -50.4 (c, 1.81 in $CHCl_3$).

*2′-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* **2′-O-trans-*Feruloylalangiside***
[173180-42-2]
$C_{35}H_{39}NO_{13}$ 681.692
Alkaloid from fruits of *Alangium lamarckii* (Alangiaceae). Amorph. powder. $[\alpha]_D^{24}$ -153 (c, 1.0 in MeOH).

*2′-(4-Hydroxy-3,5-dimethoxy-*E*-cinnamoyl):* **2′-O-trans-*Sinapoylalangiside***
[173180-45-5]
$C_{36}H_{41}NO_{14}$ 711.718
From fruits of *Alangium lamarckii* (Alangiaceae). Cryst. (H_2O). Mp 179-181°. $[\alpha]_D^{23}$ -157 (c, 1.0 in MeOH).

*2′-*O*-[4-(1,3-Dihydroxypropoxy)-3-methoxy-*E*-cinnamoyl]:* **2′-O-trans-*[4-(1,3-Dihydroxypropoxy)-3-methoxycinnamoyl]alangiside***
[173180-47-7]
$C_{38}H_{45}NO_{15}$ 755.771
From fruits of *Alangium lamarckii* (Alangiaceae). Cryst. (H_2O). Mp 166-169°. $[\alpha]_D^{27}$ -153 (c, 0.51 in MeOH).

Me ether:
Needles + 1.5 H_2O (EtOAc). Mp 236°.

O-*De-Me:* ***Demethylalangiside***
[47763-23-5]
$C_{24}H_{29}NO_{10}$ 491.494
Alkaloid from the roots of *Cephaelis ipecacuanha* (Rubiaceae) and leaves of *Alangium platanifolium* var. *trilobum* (Alangiaceae). Needles (MeOH aq.). Mp 180-182°. $[\alpha]_D^{24}$ -73 (c,0.2 in MeOH).

O-*De-Me, 2-*O*-β-*D*-glucopyranoside:*
[408363-51-9]
$C_{30}H_{39}NO_{15}$ 653.636
Alkaloid from the roots of *Cephaelis acuminata*. Amorph. powder. $[\alpha]_D^{27}$ -24 (c, 0.34 in MeOH). λ_{max} 206 (log ϵ 4.4); 231 (log ϵ 4.25); 242 (sh) (log ϵ 4.18); 280 (log ϵ 3.66) (MeOH).

O-*De-Me, 6′-(4-hydroxy-3-methoxycinnamoyl):* **6′-O-*Feruloyldemethylalangiside***
[141361-35-5 , 141434-40-4]
$C_{34}H_{37}NO_{13}$ 667.665
Alkaloid from leaves of *Alangium platanifolium* var. *trilobum* (Alangiaceae). Powder. Isol. as a mixt. of *cis*- and *trans*-forms.

O-*De-Me, 2′-(4-hydroxy-3-methoxy-*E*-cinnamoyl):* **2′-O-trans-*Feruloyldemethylalangiside***
[173180-41-1]
$C_{34}H_{37}NO_{13}$ 667.665
From fruits of *Alangium lamarckii* (Alangiaceae). Cryst. (H_2O). Mp 175-177°. $[\alpha]_D^{27}$ -162 (c, 0.44 in MeOH).

O-*De-Me, 2′-(4-hydroxy-3,5-dimethoxy-*E*-cinnamoyl):* **2′-O-trans-*Sinapoyldemethylalangiside***
[173180-44-4]
$C_{35}H_{39}NO_{14}$ 697.691
From fruits of *Alangium lamarckii* (Alangiaceae). Cryst. (H_2O). Mp 183.5-186°. $[\alpha]_D^{26}$ -155 (c, 0.43 in MeOH).

O-*De-Me, 6′-(4-hydroxy-3,5-dimethoxycinnamoyl):* **6′-*Sinapoyldemethylalangiside***
[141435-01-0 , 141361-36-6]
$C_{35}H_{39}NO_{14}$ 697.691
Alkaloid from leaves of *Alangium platanifolium* var. *trilobum* (Alangiaceae). Powder. Isol. as mixt. of *cis*- and *trans*-isomers.

O-*De-Me,* O^2-*Me:* **3-O-*Demethyl-2-*O*-methylalangiside***
[57071-85-9]
$C_{25}H_{31}NO_{10}$ 505.521
Alkaloid from fruits of *Alangium lamarckii* (Alangiaceae) and roots of *Cephaelis ipecacuanha* (Rubiaceae). Needles (MeOH aq.). Mp 275-277°. $[\alpha]_D^{26}$ -48 (c, 1.0 in MeOH).

O-*De-Me,* O^2-*Me, 2′-(4-hydroxy-3-methoxy-*E*-cinnamoyl):* **2′-O-trans-*Feruloyl-3-*O*-demethyl-2-*O*-methylalangiside***
[173180-43-3]
$C_{35}H_{39}NO_{13}$ 681.692
From fruits of *Alangium lamarckii* (Alangiaceae). Amorph. powder. $[\alpha]_D^{28}$ -115 (c, 0.43 in MeOH).

O-*De-Me,* O^2-*Me, 2′-(4-hydroxy-3,5-dimethoxy-*E*-cinnamoyl):* **2′-O-trans-*Sinapoyl-3-*O*-demethyl-2-*O*-methylalangiside***
[173180-46-6]
$C_{36}H_{41}NO_{14}$ 711.718
From fruits of *Alangium lamarckii* (Alangiaceae). Amorph. powder. $[\alpha]_D^{28}$ -126 (c, 0.39 in MeOH).

3-Demethoxy, 1-hydroxy: ***Demethylneoalangiside***
[169304-90-9]
$C_{24}H_{29}NO_{10}$ 491.494
Alkaloid from the fruits of *Alangium lamarckii*. Cryst. (MeOH aq.). Mp 193-195°. $[\alpha]_D^{28}$ -9.8 (c, 1 in MeOH). λ_{max} 231 (sh) (log ϵ 4.24); 239 (log ϵ 4.25); 287 (sh) (log ϵ 3.37) (MeOH).

3-Demethoxy, 1-hydroxy, O^2-*Me:* ***Neoalangiside***
[169391-62-2]
$C_{25}H_{31}NO_{10}$ 505.521
Alkaloid from the fruits of *Alangium lamarckii*. Amorph. powder. $[\alpha]_D^{23}$ +7.7 (c, 0.25 in MeOH). λ_{max} 230 (sh) (log ϵ 4.27); 234 (log ϵ 4.27); 286 (sh) (log ϵ 3.38) (MeOH).

*$\Delta^{8a,12a}$-Isomer, 9*R*-methoxy, 13,13*a*-didehydro:* [206875-77-6]
$C_{26}H_{31}NO_{11}$ 533.531
Alkaloid from the fruit of *Alangium lamarckii*. Pale yellow powder. $[\alpha]_D^{27}$ +8.5 (c, 1 in MeOH). λ_{max} 221 (log ϵ 4.32); 226 (log ϵ 4.32); 243 (sh) (log ϵ 4.02); 258 (sh) (log ϵ 3.79); 267 (log ϵ 3.84); 351 (log ϵ 4.33); 366 (sh) (log ϵ 4.24) (MeOH).

*$\Delta^{8a,12a}$-Isomer, 9*S*-methoxy, 13,13*a*-didehydro:* [206875-80-1]
$C_{26}H_{31}NO_{11}$ 533.531
Alkaloid from the fruit of *Alangium lamarckii*. Pale yellow needles (MeOH). Mp 219-220°. $[\alpha]_D^{20}$ -105 (c, 1 in MeOH). λ_{max} 226 (log ϵ 4.38); 244 (sh) (log ϵ 4.1); 260 (sh) (log ϵ 3.89); 266 (log ϵ 3.91); 334 (sh) (log ϵ 4.21); 351 (log ϵ 4.37); 367 (sh) (log ϵ 4.28) (MeOH).

*6′-*O*-α-*D*-Xylopyranosyl:* **6′-O-*α-D-Xylopyranosylalangiside***
[201555-41-1]
$C_{30}H_{39}NO_{14}$ 637.636
Alkaloid from the fruit of *Alangium lamarckii* (Alangiaceae). Amorph. powder. $[\alpha]_D^{29}$ -38 (c, 0.3 in MeOH). λ_{max} 233 (log ϵ 4.32); 284 (log ϵ 3.68) (MeOH).

*3′-*O*-β-*D*-Glucopyranosyl:* **3′-O-*β-D-Glucopyranosylalangiside***
[201555-37-5]
$C_{31}H_{41}NO_{15}$ 667.663
Alkaloid from the fruit of *Alangium lamarckii* (Alangiaceae). Amorph. powder. $[\alpha]_D^{26}$ -107 (c, 0.5 in MeOH). λ_{max} 233 (log ϵ 4.34); 284 (log ϵ 3.71) (MeOH).

*6′-*O*-α-*D*-Glucopyranosyl:* **6′-O-*α-D-Glucopyranosylalangiside***
[201555-38-6]
$C_{31}H_{41}NO_{15}$ 667.663
Alkaloid from the fruit of *Alangium lamarckii* (Alangiaceae). Amorph. powder. $[\alpha]_D^{26}$ -33 (c, 1 in MeOH). λ_{max} 234 (log ϵ 4.34); 284 (log ϵ 3.69) (MeOH).

*6′-*O*-β-*D*-Glucopyranosyl:* **6′-O-*β-D-Glucopyranosylalangiside***
[201555-36-4]
$C_{31}H_{41}NO_{15}$ 667.663
Alkaloid from the fruit of *Alangium lamarckii* (Alangiaceae). Amorph. powder. $[\alpha]_D^{26}$ -81 (c, 0.7 in MeOH). λ_{max} 233 (log ϵ 4.32); 284 (log ϵ 3.67) (MeOH).

*6′-*O*-α-*D*-Glucopyranosyl,* O-*de-Me,* O^2-*Me:* **6′-O-*α-D-Glucopyranosyl-3-*O*-demethyl-2-*O*-methylalangiside***
[201555-39-7]
$C_{31}H_{41}NO_{15}$ 667.663
Alkaloid from the fruit of *Alangium lamarckii* (Alangiaceae). Amorph. powder. $[\alpha]_D^{30}$ +2.4 (c, 0.7 in MeOH). λ_{max} 234 (log ϵ 4.32); 283 (log ϵ 3.65); 292 (sh) (log ϵ 3.55) (MeOH).

*13*a*-Epimer:* ***Isoalangiside***
[57128-91-3]
$C_{25}H_{31}NO_{10}$ 505.521
Alkaloid from fruits of *Alangium lamarckii* (Alangiaceae). Amorph. powder. $[\alpha]_D^{25}$ -118 (c, 0.86 in MeOH).

*13*a*-Epimer, Me ether:* ***Methylisoalangiside***
$C_{26}H_{33}NO_{10}$ 519.547
Alkaloid from fruits of *Alangium lamarckii* (Alangiaceae). Amorph. powder. $[\alpha]_D^{25}$ -141 (c, 0.28 in MeOH).

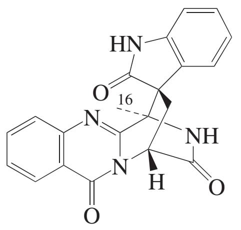
*13*a*-Epimer,* O-*de-Me:* ***Demethylisoalangiside***
[169531-70-8]
$C_{24}H_{29}NO_{10}$ 491.494
Alkaloid from the roots of *Cephaelis acuminata*. Amorph. powder. $[\alpha]_D^{27}$ -143 (c, 0.24 in MeOH). λ_{max} 234 (log ϵ 4.24); 287 (log ϵ 3.64) (MeOH).

13a-Epimer, O*-de-Me,* O^2*-Me:* ***3-O-Demethyl-2-O-methylisoalangiside***
[57128-93-5]
$C_{25}H_{31}NO_{10}$ 505.521
Alkaloid from fruits of *Alangium lamarckii* (Alangiaceae). Amorph. powder. $[\alpha]^{28}_{D}$ -169 (c, 0.45 in MeOH).

Shoeb, A. *et al., J.C.S. Perkin 1*, 1975, 1245-1248 (*isol, uv, ir, pmr, ms, struct, abs config*)
Nagakura, N. *et al., Chem. Comm.*, 1978, 896-897 (*cmr*)
Höfle, G. *et al., Chem. Ber.*, 1980, **113**, 566-576 (*synth, uv, ir, pmr, cmr, ms*)
Itoh, A. *et al., Phytochemistry*, 1991, **30**, 3117-3123; 1992, **31**, 1037-1040; 1994, **36**, 383-387 (*Demethylalangiside, 6′-O-Feruloyldemethylalangiside, 6′-O-Sinapoyldemethylalangiside, 3-O-Demethyl-2-O-methylalangiside*)
Itoh, A. *et al., J. Nat. Prod.*, 1995, **58**, 1228-1239 (*Isoalangiside, Methylisoalangiside, 3-O-Demethyl-2-O-methylisoalangiside, Neoalangiside, Demethylneoalangiside*)
Itoh, A. *et al., Phytochemistry*, 1996, **41**, 651-656; 1997, **46**, 1225-1229 (*esters, glycosyl derivs*)
Itoh, A. *et al., Heterocycles*, 1998, **48**, 499-505 (*9-methoxy derivs*)
Itoh, A. *et al., Phytochemistry*, 2002, **59**, 91-97 (*Demethylisoalangiside, O-de-Me glucoside*)

Alantrypinone A-240

PF 1198A. Antibiotic PF 1198A



(+)-*form*

$C_{21}H_{16}N_4O_3$ 372.382

(+)-*form* [212911-06-3]
Prod. by *Aspergillus terreus* PF1198 and *Penicillium thymicola*. Mycotoxin. Insecticidal agent. Amorph. solid. $[\alpha]^{22}_{D}$ +37 (c, 2.1 in EtOH). λ_{max} 210 (log ϵ 3.78); 257 (log ϵ 3.15); 266 (log ϵ 3.17); 277 (log ϵ 3.08); 292 (log ϵ 2.73); 303 (log ϵ 2.77); 316 (log ϵ 2.62) (EtOH).

16-Hydroxy: ***(-)-Serantrypinone***
[956006-97-6]
$C_{21}H_{16}N_4O_4$ 388.382
Prod. by *Penicillium thymicola*. Mp > 240°. $[\alpha]^{22}_{D}$ -12 (c, 0.12 in EtOH). λ_{max} 218 (log ϵ 4.55); 267 (log ϵ 3.54); 278 (log ϵ 3.51); 290 (log ϵ 3.36); 305 (log ϵ 3.16); 318 (log ϵ 3.05) (EtOH).

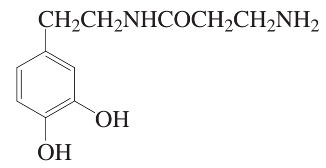
(-)-*form*

16-Hydroxy: ***(+)-Serantrypinone****. Antibiotic PF 1198B. PF 1198B*
[366785-28-6]
$C_{21}H_{16}N_4O_4$ 388.382
Prod. by *Aspergillus terreus* PF 1198. Mp > 250°. $[\alpha]_{D}$ +21.7 (c, 0.1 in MeOH). λ_{max} 208 ; 258 ; 266 ; 278 ; 303 ; 315 (MeOH).

Larsen, T.O. *et al., J. Nat. Prod.*, 1998, **61**, 1154-1157 (*isol, uv, pmr, cmr, cryst struct, abs config*)
Ariza, M.R. *et al., J. Nat. Prod.*, 2001, **64**, 1590-1592 (*Serantrypinone*)
Hart, D.J. *et al., J.A.C.S.*, 2001, **123**, 5892-5899 (*synth, abs config*)
Kuriyama, T. *et al., J. Agric. Food Chem.*, 2004, **52**, 3884-3887 (*isol, pmr, cmr*)
Chen, Z. *et al., J.O.C.*, 2004, **69**, 79-85 (*synth*)
Hart, D.J. *et al., Tet. Lett.*, 2007, **48**, 7069-7071 (*Serantrypinone, synth, abs config*)

N-β-Alanyldopamine A-241

*3-Amino-*N*-[2-(3,4-dihydroxyphenyl)ethyl]propanamide, 9CI*
[54653-62-2]
[58077-93-3]



$C_{11}H_{16}N_2O_3$ 224.259
Occurs in insects. Precursor to sclerotized insect cuticle; functions as cross-linking agent between peptide chains. No phys. props. reported.

*3-*O*-β-*D*-Glucopyranoside:* [96735-97-6]
$C_{17}H_{26}N_2O_8$ 386.401
Occurs in insects. Precursor in insect cuticule sclerotization.

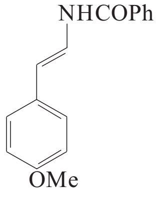
*4-*O*-β-*D*-Glucopyranoside:* [96848-78-1]
$C_{17}H_{26}N_2O_8$ 386.401
Isol. from *Manduca sexta* insects. No phys. props. reported.

N*-Ac, 3-*O*-β-*D*-glucopyranoside:* [88874-85-5]
$C_{19}H_{28}N_2O_9$ 428.438
Isol. from praying mantis *Hierodula patellifera*, *Manduca sexta* and *Mantis religiosa*. No phys. props. reported.

Hopkins, T.L. *et al., Science (Washington, D.C.)*, 1982, **217**, 364-366 (*isol, synth, biochem*)
Yago, M. *et al., Insect Biochem.*, 1984, **14**, 7-9; 487-489 (*N-Ac glucoside*)
Mueller, D.D. *et al., Bioconjug. Chem.*, 1993, **4**, 47-53 (*cmr, pmr*)
Hopkins, T.L. *et al., Insect Biochem. Mol. Biol.*, 1995, **25**, 29-37 (*3-glucoside*)
Merritt, M.E. *et al., J.A.C.S.*, 1996, **118**, 11278-11282 (*props*)

Alatamide A-242

N*-[2-(4-Methoxyphenyl)ethenyl]benzamide, 9CI.* N*-(*p*-Methoxystyryl)benzamide*



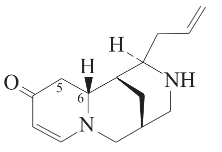
$C_{16}H_{15}NO_2$ 253.3

(*E*)-*form* [54797-23-8]
Obt. from leaves of *Pleiospermium alatum* (Rutaceae) and aerial parts of *Piper guayranum* (Piperaceae). Cryst. (C_6H_6/$CHCl_3$), granular cryst. (CH_2Cl_2/petrol), flakes (MeOH/$CHCl_3$). Mp 169° Mp 178-180° Mp 190-193°. Although thought to be principally the (*E*)-form, Mp variations may be the result of config. inhomogeneity.

Galat, A. *et al., J.A.C.S.*, 1950, **72**, 4436 (*synth*)
Chatterjee, A. *et al., Aust. J. Chem.*, 1975, **28**, 457 (*isol, ir, uv, ms*)
Ghosh, S. *et al., Synth. Commun.*, 1987, **17**, 299 (*synth, ir*)
Maxwell, A. *et al., J. Nat. Prod.*, 1989, **52**, 411 (*isol, uv, ir, pmr, ms*)

Albine A-243

Dehydroalbine
[53915-26-7]



Absolute configuration

$C_{14}H_{20}N_2O$ 232.325
Alkaloid from *Lupinus albus* and *Lupinus termis* seeds (Fabaceae). Mp 50°. $[\alpha]^{25}_{D}$ -103. The *N*-Methyl deriv. was formerly reported erroneously (see Alkaloid LC2, A-554).

Perchlorate: Mp 253°. $[\alpha]^{25}_{D}$ -76 (H_2O).

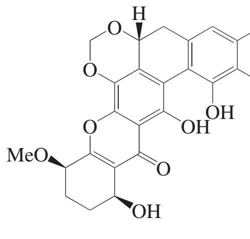
N*-Formyl:* ***N-Formylalbine***
$C_{15}H_{20}N_2O_2$ 260.335
Trace alkaloid in seeds and leaves of *Lupinus albescens* (Fabaceae). Provisional identification.

5,6-Didehydro: ***Δ^5-Dehydroalbine***
$C_{14}H_{18}N_2O$ 230.309
Alkaloid from seeds of *Lupinus termis* (Fabaceae). Oil. $[\alpha]^{25}_{D}$ -44.6 (c, 0.02 in MeOH).

Wiewiórowski, M. *et al., Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1964, **12**, 213; 217 (*isol, ir*)
Chekhlov, A.N. *et al., J. Struct. Chem. (Engl. Transl.)*, 1974, **15**, 848 (*cryst struct*)
Wolńska-Mocydlarz, J. *et al., Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1976, **24**, 613 (*ir, struct*)
Mohamed, M.H. *et al., Phytochemistry*, 1991, **30**, 3111 (*Δ^5-Dehydroalbine*)
Planchuelo-Ravelo, A.M. *et al., Z. Naturforsch., C*, 1993, **48**, 414 (*N-Formylalbine*)

Albofungin A-244

Kanchanomycin. BA 180265A. P 42-1. Antibiotic P 42-1
[37895-35-5]



Absolute Configuration

$C_{27}H_{24}N_2O_9$ 520.495
Stereochem. revised in 1992. Metab. of *Actinomyces albus* var. *fungatus* and *Actinomyces tumemacerans*. Antifungal agent with antineoplastic props. Yellow cryst. ($MeNO_2$). Mp 304-307°. $[\alpha]^{20}_{D}$ -670

(DMF). Log P 0.34 (uncertain value) (calc). λ_{max} 250 (ϵ 9000); 320 (ϵ 5000); 388 (ϵ 8000) (MeOH/NaOH) (Derep). λ_{max} 230 (ϵ 36400); 253 (ϵ 36500); 300 (ϵ 14600); 364 (sh) (ϵ 22400); 373 (ϵ 23700) (MeOH) (Derep).

▶ LD_{50} (mus, ipr) 2 mg/kg. ZD5706000

Penta-Ac: Mp 230-233°.

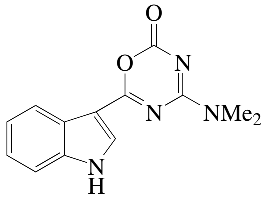
4-Chloro: ***Chloroalbofungin***. *Albofungin B*
[37891-66-0]
$C_{27}H_{23}ClN_2O_9$ 554.939
From *Actinomyces albus* var. *fungatus* and from *Streptomyces* spp. Possesses antifungal and antineoplastic activities. Cryst. ($MeNO_2$). Sol. Me_2CO, DMF, DMSO, Py, $CHCl_3$, dioxan, AcOH; fairly sol. MeOH, EtOH, $CHCl_3$, C_6H_6, butanol; poorly sol. H_2O, Et_2O, hexane. Mp 327-330°. $[\alpha]_D^{20}$ -560 (DMF). Log P 1.27 (uncertain value) (calc). λ_{max} 230 (E1%/1cm 530); 257 (E1%/1cm 540); 311 (E1%/1cm 330); 365 (E1%/1cm 320) (MeOH) (Berdy). λ_{max} 233 (ϵ 26300); 254 (ϵ 31600); 305 (ϵ 12300); 384 (ϵ 20900) (EtOH) (Berdy).

Gurevich, A.I. *et al., Tet. Lett.*, 1972, **13**, 1751-1754; 1974, **15**, 2801 (*Albofungin, Chloroalbofungin, isol, uv, pmr*)
Fukushima, K. *et al., J. Antibiot.*, 1973, **26**, 65-69 (*P42-1*)
Kogan, G.A. *et al., J. Struct. Chem. (Engl. Transl.)*, 1975, **15**, 793-799 (*cd*)
Onoprienko, V.V. *et al., Bioorg. Khim.*, 1978, **4**, 1418-1422 (*struct*)
Cooper, R. *et al., J. Antibiot.*, 1992, **45**, 444-453 (*pmr, cmr, stereochem, abs config*)

Alboinone

A-245

*4-(Dimethylamino)-6-(1*H*-indol-3-yl)-2*H*-1,3,5-oxadiazin-2-one, 9CI*
[188547-40-2]



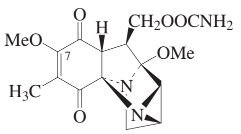
$C_{13}H_{12}N_4O_2$ 256.263
First naturally occurring oxadiazinone. Alkaloid from the ascidian *Dendrodoa grossularia*. λ_{max} 210 ; 252 ; 270 ; 334 (MeOH).

Bergmann, T. *et al., Tetrahedron*, 1997, **53**, 2055-2060 (*isol, uv, ir, pmr, cmr, ms, struct, synth*)

Albomitomycin A

A-246

Antibiotic AX 1
[110934-24-2]



Absolute Configuration

$C_{16}H_{19}N_3O_6$ 349.343

Quinone antibiotic. Metab. of *Streptomyces caespitosus*. Prod. by intramolecular rearrangement of Mitomycin A, M-653. Plates ($CHCl_3$). $[\alpha]_D^{23}$ -2.7 (c, 0.5 in $CHCl_3$). Dec. at >130°. λ_{max} 215 (ϵ 3300); 288 (ϵ 10000) (MeOH) (Berdy).

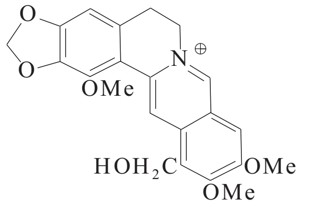
7-Demethoxy, 7-amino: ***Albomitomycin C***
[111750-67-5]
$C_{15}H_{18}N_4O_5$ 334.331
From *Streptomyces* sp. Prisms. Mp 120° dec. $[\alpha]_D^{26}$ +34.7 (c, 0.3 in $CHCl_3$). Incorrect MF given in paper. λ_{max} 242 (ϵ 5012); 344 (ϵ 6310) (MeOH) (Berdy).

Fukuyama, T. *et al., Tet. Lett.*, 1986, **27**, 6299 (*synth*)
Kono, M. *et al., J.A.C.S.*, 1987, **109**, 7224 (*isol, struct*)
Hirayama, N. *et al., Acta Cryst. C*, 1991, **47**, 409 (*cryst struct*)
Kono, M. *et al., J. Antibiot.*, 1995, **48**, 179 (*Albomitomycin C, isol, pmr, cmr, uv*)

Alborine

A-247

Pangrenine. Alkaloid PO5. Alkaloid R-K
[23943-91-1]



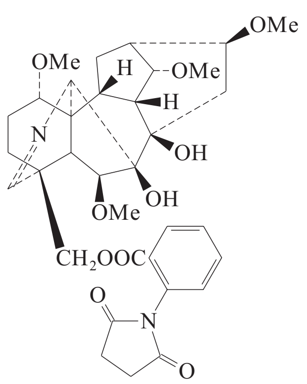
$C_{22}H_{22}NO_6^{\oplus}$ 396.419
Alkaloid from *Papaver pseudocanescens, Papaver oreophilum, Papaver nudicaule* var. *leiocarpum, Papaver pyrenaicum, Papaver alboroseum* and *Papaver angrenicum*. Yellow needles (MeOH)(as iodide or perchlorate). Mp 255-258° dec. (sinters from 228°)(as perchlorate) Mp 281-283° (as nitrate).

Preininger, V. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 124; 1440 (*uv, pmr, struct, bibl*)
Pfeifer, S. *et al., Pharmazie*, 1972, **27**, 48
Novák, V. *et al., Coll. Czech. Chem. Comm.*, 1974, **39**, 883 (*isol*)
Siddikov, D. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 442-445 (*isol, cryst struct*)

Alboviolaconitine D

A-248

[138842-68-9]



$C_{34}H_{42}N_2O_{10}$ 638.713

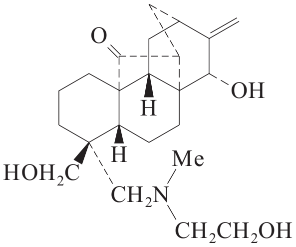
Alkaloid from roots of *Aconitum alboviolaceum* (Ranunculaceae).

Chen, D. *et al., Huaxue Xuebao*, 1992, **50**, 1211; *CA*, **118**, 230146m

Albovionitine

A-249

[138935-81-6]



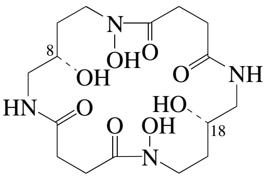
$C_{23}H_{35}NO_4$ 389.534
Alkaloid from *Aconitum alboviolaceum*. Cryst. ($CHCl_3$). Mp 150-152°.

Zhigang, H. *et al., Phytochemistry*, 1991, **30**, 3494-3496 (*isol, pmr, cmr, ms*)

Alcaligin

A-250

1,8,11,18-Tetrahydroxy-1,6,11,16-tetraazacycloeicosane-2,5,12,15-tetrone, 9CI
[117959-43-0]



$C_{16}H_{28}N_4O_8$ 404.419
Isol. from *Alcaligenes denitrificans* ssp. *xylosoxydans, Bordetella pertussis* and *Bordetella bronchiseptica*. Siderophore. Cryst. + $2H_2O$ (H_2O). $[\alpha]_D^{27}$ +40.4 (c, 0.54 in MeOH). λ_{max} 206 ; 426 (H_2O) (Berdy).

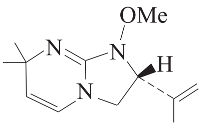
8,18-Dideoxy: 1,11-Dihydroxy-1,6,11,16-tetraazacycloeicosane-2,5,12,15-tetrone, 9CI. ***Putrebactin***
[188944-66-3]
$C_{16}H_{28}N_4O_6$ 372.42
Prod. by *Shewanella putrefaciens*. Siderophore.

Nishio, T. *et al., J.A.C.S.*, 1988, **110**, 8733 (*isol, struct*)
Nishio, T. *et al., Agric. Biol. Chem.*, 1990, **54**, 1837 (*isol*)
Bergeron, R.J. *et al., J.O.C.*, 1991, **56**, 5560 (*synth*)
Moore, C.H. *et al., J. Bacteriol.*, 1995, **177**, 1116 (*isol*)
Ledyard, K.M. *et al., J. Biol. Inorg. Chem.*, 1997, **2**, 93-97 (*Putrebactin*)

Alchorneine

A-251

*1,2,3,7-Tetrahydro-1-methoxy-7,7-dimethyl-2-(1-methylethenyl)imidazo[1,2-*a*]pyrimidine, 9CI*



Absolute configuration

$C_{12}H_{19}N_3O$ 221.302

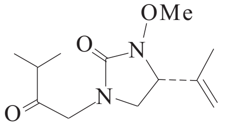
***(R)*-form** [28340-21-8]
Alkaloid from *Alchornea floribunda* and *Alchornea hirtella* (Euphorbiaceae). Effective as a spasmolytic agent in dogs. Ganglioplegic parasympathomimetic agent. Strong vagolytic agent and inhibitor of intestinal peristalsis. Mp 43°. $[\alpha]_D$ -105 (c, 1 in $CHCl_3$).

Methiodide:
Cryst. (Me_2CO/MeOH). Mp 159°. $[\alpha]_D$ -28 (EtOH).

Cesario, M. *et al., Acta Cryst. B*, 1972, **28**, 151 (*cryst struct*)
Fr. Pat., 1972, 2 087 982; *CA*, **77**, 88757a (*isol, use*)
Khuong-Huu, F. *et al., Tetrahedron*, 1972, **28**, 5207 (*isol, ir, uv, pmr, ms, struct, abs config*)
Büchi, G. *et al., J.O.C.*, 1989, **54**, 4494 (*synth*)

Alchorneinone A-252

[41758-41-2]

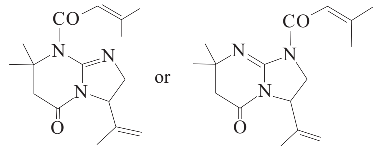


$C_{12}H_{20}N_2O_3$ 240.302
Alkaloid from the leaves of *Alchornea floribunda* (Euphorbiaceae). Liq. $[\alpha]_D$ -66 (c, 1 in $CHCl_3$).

Khuong-Huu, F. *et al., Tetrahedron*, 1972, **28**, 5207 (*isol, ir, pmr, ms, struct*)

Alchornidine A-253

[25801-15-4]



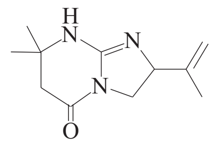
Preferred structure

$C_{16}H_{23}N_3O_2$ 289.377
Spectroscopic data do not allow a firm choice to be made between two alternative structs. Minor alkaloid from the leaves of *Alchornea javanensis* (Euphorbiaceae). Glistening needles by subl. Mp 96-97°. $[\alpha]_D$ -18 (c, 1.1 in $CHCl_3$).

Hart, N.K. *et al., Aust. J. Chem.*, 1970, **23**, 1679-1693 (*isol, ir, pmr, ms, struct*)

Alchornine A-254

[25819-91-4]



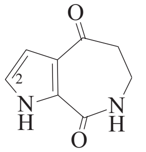
$C_{11}H_{17}N_3O$ 207.275
A major constit. of both the leaves and bark of *Alchornea javanensis* (Euphorbiaceae). Needles (petrol/C_6H_6). Mp 134-135°. $[\alpha]_D$ +74 (c, 1.5 in $CHCl_3$).

Picrate:
Yellow prisms (EtOH). Mp 275-278°.

Hart, N.K. *et al., Aust. J. Chem.*, 1970, **23**, 1679 (*isol, ir, pmr, ms, struct*)

Aldisine A-255

*6,7-Dihydropyrrolo[2,3-*c*]azepine-4,8(1*H*,5*H*)-dione, 9CI*
[72908-87-3]



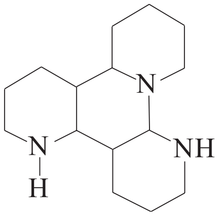
$C_8H_8N_2O_2$ 164.163
Isol. from the marine sponges *Hymeniacidon aldis*, *Axinella carteri* and *Pseudaxinyssa cantharella*. Mp 275-277° (269° dec.). $[\alpha]_D$ -6 (c, 0.12 in MeOH). λ_{max} 216 (ϵ 19100); 245 (ϵ 8370); 295 (ϵ 6770) (MeOH) (Derep).

2-Bromo: ***2-Bromoaldisine***
[96562-96-8]
$C_8H_7BrN_2O_2$ 243.059
Isol. from *Hymeniacidon aldis*, an unidentified sponge from Fiji, a *Lissodendoryx* sp. of sponge from Sri Lanka and from *Pseudaxinyssa cantharella*. Cryst. (MeOH). Mp 265° (243°). $[\alpha]_D$ +5 (c, 0.47 in MeOH). λ_{max} 220 (ϵ 29600); 244 (sh) (ϵ 12100); 303 (ϵ 8130) (MeOH) (Derep).

Sharma, G.M. *et al., Chem. Comm.*, 1980, 435 (*synth, uv, pmr, cmr*)
Schmitz, F.J. *et al., J. Nat. Prod.*, 1985, **48**, 47 (*isol, uv, ir, pmr, cmr, ms, struct, deriv*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1985, **21**, 578; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 547 (*isol*)
De Nanteuil, G. *et al., Tetrahedron*, 1985, **41**, 6019 (*isol, uv, ir, pmr, cmr, ms, cd, deriv*)
Xu, X.-H. *et al., J. Struct. Chem. (Engl. Transl.)*, 2001, **20**, 173-175 (*cryst struct*)

α-Aldotripiperideine A-256

[642-10-4]



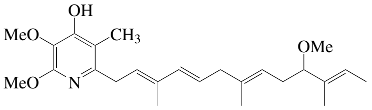
$C_{15}H_{27}N_3$ 249.398
Alkaloid from *Coelidium fourcadei* dried branches and leaves (Fabaceae). Cryst. (hexane). Mp 121° (115-118°). Prob. an artifact of thermal dec.

Schöpf, C. *et al., Angew. Chem.*, 1950, **62**, 452 (*synth*)

Arndt, R.R. *et al., J. S. Afr. Chem. Inst.*, 1968, **21**, 54; *CA*, **70**, 4342f (*isol*)

Aleicide B A-257

2,3-Dimethoxy-6-(10-methoxy-3,7,11-trimethyl-2,4,7,11-tridecatetraenyl)-5-methyl-4-pyridinol, 9CI
[156204-42-1]



$C_{25}H_{37}NO_4$ 415.572
Prod. by *Streptomyces aurantiacus*. Insecticide.

Shopotova, L.P. *et al., Zh. Prikl. Khim. (Leningrad)*, 1993, **66**, 1111-1117 (*isol, pmr, cmr, ms*)

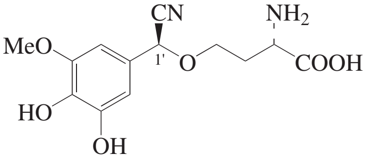
Aleicide C A-258

$C_{25}H_{37}NO_5$ 431.571
Prod. by *Streptomyces aurantiacus*. Insecticide.

Navashin, S.M. *et al., Antibiotiki (Moscow)*, 1994, **39**, 3-12

Aleurodisconitrile A-259

[1000180-33-5]



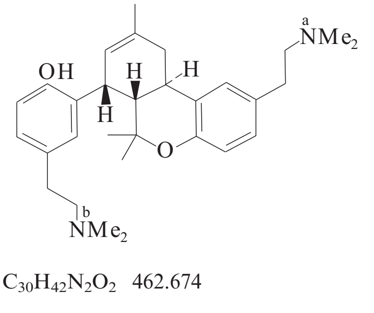
$C_{13}H_{16}N_2O_6$ 296.279
Isol. from the fruiting bodies of *Aleurodiscus amorphus*. Solid. λ_{max} 212 (log ϵ 4.07); 246 (log ϵ 3.31); 274 (log ϵ 2.79) (MeOH).

Decyano, 1′-oxo: ***Aleurodiscoester***
[1000180-34-6]
$C_{12}H_{15}NO_7$ 285.253
Isol. from fruiting bodies of *Aleurodiscus amorphus*. Solid. $[\alpha]_D^{25}$ +70 (c, 0.13 in MeOH). λ_{max} 217 (log ϵ 3.57); 277 (log ϵ 3.18) (MeOH).

Kindler, B.L.J. *et al., Angew. Chem., Int. Ed.*, 2007, **46**, 8076-8078 (*isol, cd, pmr, cmr*)

Alfileramine A-260

[73326-84-8]



$C_{30}H_{42}N_2O_2$ 462.674

A bishordeninylterpene alkaloid related structurally to the cannabinoids. Exists in soln. as an equilib. mixt. of 2 rotamers. Alkaloid from the leaves of *Zanthoxylum punctatum*, *Zanthoxylum chiriquinum* and *Zanthoxylum coriaceum* (Rutaceae). Mp 185-187°. Opt. inactive.

Methiodide (1:2): Mp 253-255°.

N^a-*De-Me:* ***N^a-Demethylalfileramine***
[129743-97-1]
$C_{29}H_{40}N_2O_2$ 448.647
Alkaloid from the leaves of *Zanthoxylum coriaceum* (Rutaceae). Opt. inactive.

N^b-*De-Me:* ***N^b-Demethylalfileramine***
[129743-98-2]
$C_{29}H_{40}N_2O_2$ 448.647
Alkaloid from the leaves of *Zanthoxylum coriaceum* (Rutaceae). Opt. inactive.

N^a,N^b-*Di-de-Me:* ***N^a,N^b-Didemethylalfileramine***
[129743-95-9]
$C_{28}H_{38}N_2O_2$ 434.62
Alkaloid from the leaves of *Zanthoxylum coriaceum* (Rutaceae). Amorph. Opt. inactive.

Me ether: **O-*Methylalfileramine***
[128700-82-3]
$C_{31}H_{44}N_2O_2$ 476.701
Alkaloid from the leaves of *Zanthoxylum chiriquinum* (Rutaceae). Oil (solidifies upon standing). Opt. inactive.

Caolo, M.A. *et al., Tetrahedron*, 1979, **35**, 1487-1492 (*isol, uv, ir, pmr, ms, cryst struct*)
Swinehart, J.A. *et al., Phytochemistry*, 1980, **19**, 1219-1223 (*isol*)
Marcos, M. *et al., Tetrahedron*, 1989, **45**, 7477-7484 (*uv, ir, pmr, cmr, ms*)
Marcos, M. *et al., J. Nat. Prod.*, 1990, **53**, 459-461 (*O-Methylalfileramine*)
Marcos, M. *et al., Phytochemistry*, 1990, **29**, 2315-2319 (*Demethylalfileramines*)

Alginidine A-261

[1353-94-2]

Struct. unknown

$C_{27}H_{43}NO_4$ 445.641

Steroidal alkaloid. Alkaloid from *Fritillaria severzowii* (Liliaceae). Mp 164°. $[\alpha]_D$ -24.6 (MeOH).

Hydrochloride: Mp 230-232°.

Methiodide: Mp 288-289°.

Nuriddinov, R.N. *et al., CA*, 1962, **57**, 15165

Alginine† A-262

$C_{23}H_{39}NO_3$ 377.566

Steroidal alkaloid of unknown struct. contg. 3 OH groups. Alkaloid from *Fritillaria severzowii* (Liliaceae). CNS stimulant, adrenergic blocking agent, local anaesthetic. Mp 271-272°. $[\alpha]_D$ +108.5.

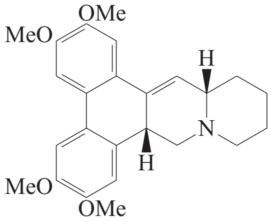
Hydrochloride: Mp 323-325°.

Methiodide: Mp 310-311°.

Yunusov, S. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1939, **9**, 1911; *CA*, **34**, 4070

Alihirsutine A A-263

[147526-80-5]

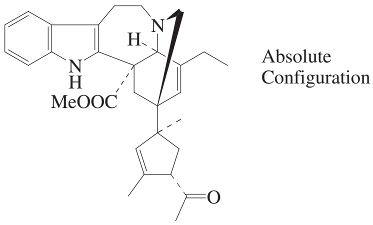


$C_{25}H_{29}NO_4$ 407.508

Alkaloid from aerial parts of *Tylophora hirsuta* (Asclepiadaceae). Cryst. ($CHCl_3$/MeOH 1:1). Mp 296-298°.

Ali, M. *et al., Fitoterapia*, 1992, **63**, 243 (*isol, uv, ir, pmr, ms, struct*)

Alioline A-264



$C_{30}H_{36}N_2O_3$ 472.626

Unusual iboga-type alkaloid containing an additional C_9 terpenoid unit, the origin of which is unclear. Alkaloid from *Catharanthus roseus.* $[\alpha]_D^{24}$ +105.5 (MeOH). λ_{max} 227 (log ε 4.13); 283 (log ε 3.69); 292 (log ε 3.61) (MeOH).

Habib-ur-Rahman, *et al., Z. Naturforsch., B*, 2005, **60**, 870-874 (*isol, pmr, cmr*)

Aconitum nemorosum C_{20} Alkaloid A-265

$C_{20}H_{25}NO_3$ 327.422

Struct. unknown. Alkaloid from *Aconitum nemorosum*. Cryst. (Me_2CO). Mp 244-246°. Could be identical with Hetisinone (see under Hetisan-2,11,13-triol, H-202.

Monakhova, T.E. *et al., Khim. Prir. Soedin.*, 1965, **1**, 113; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 88

Aconitum nemorosum C_{23} Alkaloid A-266

$C_{23}H_{29}NO_6$ 415.485

Struct. unknown. Alkaloid from *Aconitum nemorosum*. Mp 270-272° (as hydrochloride). MF erroneously given as $C_{23}H_{29}NO_3$ in ref. Anal. figures given correspond to O_6.

Monakhova, T.E. *et al., Khim. Prir. Soedin.*, 1965, **1**, 113; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 88

Erythrophleum C_{24} Alkaloid A-267

$C_{24}H_{37}NO_7$ 451.559

Struct. unknown. Alkaloid from the bark of *Erythrophleum chlorostachys* (Fabaceae). Glass.

Hydrochloride:
Needles (EtOH/EtOAc). Mp 191° (solvate).

3-Ac: ***C_{24} Amine 3β-acetate***
$C_{26}H_{39}NO_8$ 493.596
Alkaloid from the bark of *Erythrophleum chlorostachys* (Fabaceae).

C_{24} amide (rearrangement product):
Cryst. (EtOAc). Mp 186°. Obt. by treating the C_{24} amine with 5*M* NaOH.

Falkiner, M.J. *et al., Aust. J. Chem.*, 1975, **28**, 645-650 (*isol, pmr*)

Aconitum kirinense Alkaloid A-268

$C_{26}H_{41}NO_8$ 495.612

Struct. unknown. Isol. from *Aconitum kirinense*. Mp 134.5° (as nitrate). Conts. 4 OH, 3 OMe and 1 NMe groups.

Monakhova, T.E. *et al., Khim. Prir. Soedin.*, 1965, **1**, 113-116; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 88

Aconitum koreanum Alkaloid A-269

$C_{35}H_{41}NO_{10}$ 635.71

Struct. unknown. Isol. from *Aconitum koreanum*. Mp 210° (as hydrobromide). $[\alpha]_D^{27}$ -18.7 (c, 4.27 in EtOH). Species name given as coreanum in the English-language translation of the paper. No further reports to 2007. Later investigations of this species do not refer.

Monakhova, T.E. *et al., Khim. Prir. Soedin.*, 1965, **1**, 113-116; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 88-90
Kao, H.C. *et al., Yaoxue Xuebao*, 1966, **13**, 186-194; *CA*, **65**, 3922g (*Aconitum koreanum constits*)

Alstonia constricta Alkaloid A-270

Struct. unknown

$C_{43}H_{50}N_4O_7$ 734.891

Bisindole alkaloid. Alkaloid from the root bark of *Alstonia constricta* (Apocynaceae). Needles (Me_2CO). Mp 196-197°. $[\alpha]_D$ +9 (c, 3.3 in $CHCl_3$).

Crow, W.D. *et al., Aust. J. Chem.*, 1970, **23**, 2489-2501 (*isol, uv, ir, pmr*)

Ammodendron karelinii Alkaloid A-271

Struct. unknown

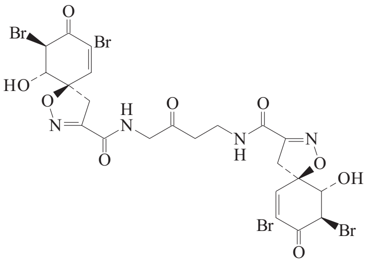
$C_{15}H_{24}N_2O$ 248.367

Quinolizidine alkaloid, prob. of Sparteine group. Alkaloid from *Ammodendron karelinii* (Fabaceae). Oil.

Kushmuradov, Yu.K. *et al., Khim. Prir. Soedin.*, 1977, **13**, 717-718; *Chem. Nat. Compd. (Engl. Transl.)*, 604-605 (*isol*)

Aplysina archeri Alkaloid A-272

[179523-37-6]



$C_{22}H_{20}Br_4N_4O_9$ 804.037

Probable abs. config. illus. Metab. from the Caribbean sponge *Aplysina archeri*. Shows antifungal activity. λ_{max} 252 (ϵ 7850) (MeOH).

Ciminiello, P. *et al., Tetrahedron*, 1996, **52**, 9863 (*isol, uv, ir, pmr, cmr, cd, struct*)

Artemisia rutifolia Alkaloid A-273

$C_{22}H_{31}NO_8$ 437.489

Struct. unknown. Isol. from epigeal parts of *Artemisia rutifolia*. Amorph. solid. Mp 189-190°. Prob. artifact (NH_3 used in extraction). *Artemisia* is not an alkaloid-bearing genus.

Brutko, L.I. *et al., Khim. Prir. Soedin.*, 1967, **3**, 292; *Chem. Nat. Compd. (Engl. Transl.)*, 1967, **3**, 247

Astragalus berterianus Alkaloid A-274

Struct. unknown. Alkaloid from *Astragalus berterianus* (Fabaceae). Mp 210°.

Gutierrez, C.P. *et al., An. Fac. Quim. Farm. (Univ. Chile)*, 1960, **12**, 120; *CA*, **56**, 5121h

Buxus Alkaloid 1 A-275

Struct. unknown. Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 199°. $[\alpha]_D$ +31 ($CHCl_3$). Props. similar to Buxaminol E in B-456 and *Buxus* Alkaloid B398, A-398.

Stauffacher, D. *et al., Helv. Chim. Acta*, 1964, **47**, 968-981 (*isol*)

Buxus Alkaloid 2 A-276

Struct. unknown. Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 195°. $[\alpha]_D$ +92 ($CHCl_3$).

Stauffacher, D. *et al., Helv. Chim. Acta*, 1964, **47**, 968-981 (*isol*)

Buxus Alkaloid 3 A-277

Struct. unknown. Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 281°. $[\alpha]_D$ +68 ($CHCl_3$).

Stauffacher, D. *et al., Helv. Chim. Acta*, 1964, **47**, 968-981 (*isol*)

Buxus Alkaloid 4 A-278

Struct. unknown. Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 177°. $[\alpha]_D$ +147 ($CHCl_3$). Props. corresp. to Buxtauine M, B-482.

Stauffacher, D. *et al., Helv. Chim. Acta*, 1964, **47**, 968-981 (*isol*)

Buxus Alkaloid 5 A-279

Struct. unknown. Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 156°. $[\alpha]_D$ +40 ($CHCl_3$).

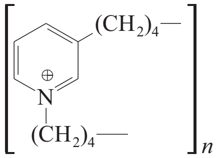
Stauffacher, D. *et al., Helv. Chim. Acta*, 1964, **47**, 968-981 (*isol*)

C-Alkaloid I A-280

Minimum formula. Struct. unknown. Alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). Prisms (Me_2CO aq.) (as picrate). Mp 194° (picrate). Blue-violet col. with $Ce(SO_4)_2$, becoming carmine on standing.

Kebrle, J. *et al., Helv. Chim. Acta*, 1953, **36**, 102-121; 1384-1386 (*isol*)

Callyspongia fibrosa Alkaloid A-281



High molecular weight oligomer or polymer. Alkaloid from the Micronesian sponge *Callyspongia fibrosa*. Inhibitor of the epidermal growth factor receptor.

Davies-Coleman, M.T. *et al., J.O.C.*, 1993, **58**, 5925

Chamaecytisus Alkaloid A-282

$C_{12}H_{20}N_2O$ 208.303

Struct. unknown. Alkaloid from *Chamaecytisus austriacus stefanoffi, Chamaecytisus ciliatus* and *Chamaecytisus polytrichus polytrichus* (Fabaceae). Mp 168-170°. Ir 1675 cm^{-1}. Prob. a tertiary amide.

Deili, A. *et al., Farmatsiya (Sofia)*, 1977, **27**, 15-18; *CA*, **89**, 56427z (*isol*)

Colchicum luteum Alkaloid A-283

$C_{19}H_{23}NO_4$ 329.395

Struct. unknown. Alkaloid from *Colchicum luteum* (Liliaceae). Mp 237-238°.

Chommadov, B. *et al., Khim. Prir. Soedin.*, 1985, 810; *Chem. Nat. Compd. (Engl. Transl.)*, 770-773 (*isol, ir, pmr, ms*)

Crotalaria retusa Alkaloid A-284

Struct. unknown. Isol. from *Crotalaria retusa*. Cryst. (Me_2CO). Mp 130-132°.

Culvenor, C.C.J. *et al., Aust. J. Chem.*, 1957, **10**, 464-473 (*isol*)

Cytisus laburnum Alkaloid A-285

$C_{12}H_{22}N_2O$ 210.319

Struct. unknown. Pyrrolizidine alkaloid. Alkaloid from *Cytisus laburnum (Laburnum laburnum)* (Fabaceae). Mp 128-129°. $[\alpha]_D^{19}$ +18.6 (EtOH). Prob. conts. one NH (?lactam) group, no NMe group.

Galinovsky, F. *et al., Sci. Pharm.*, 1953, **21**, 256; *CA*, **49**, 6977

Cytisus ruthenicus Alkaloid A-286

$C_{15}H_{16}N_2O_5$ 304.302

Prob. a quinolizidine (Sparteine-group) alkaloid. Struct. unknown. Alkaloid from *Cytisus ruthenicus* (Fabaceae). Mp 171.5-173°. $[\alpha]_D^{18}$ -15.26. Conts. *N*-Me group. Co-occurs with Sparteine.

Hydroiodide: Mp 231-233°.

Perchlorate: Mp 198-200°.

Dipicrate: Mp 199-201°.

Alekseev, V.S. *et al., Farm. Zh. (Kiev)*, 1967, **22**, 59-60; *CA*, **67**, 54325m (*isol*)

Dendrobates Alkaloid 185 A-287

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates auratus* (Dendrobatidae). Mol. formula not known; m/e 185 (1), 170 (100). Cannot be hydrogenated.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 197 A-288

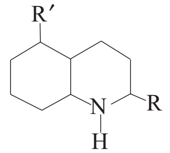
Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates auratus* (Dendrobatidae). Mol. formula not known; m/e 197 (1), 180 (100), 126 (35). Cannot be hydrogenated.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 203 A-289

Decahydro-2-(2-penten-4-ynyl)quinoline



$R = CH_2CH{=}CHC{\equiv}CH,\ R' = H$

$C_{14}H_{21}N$ 203.327

Tentative struct. A major alkaloid in skin extracts of *Dendrobates fulguritus*, trace constit. in *Dendrobates auratus, Dendrobates histrionicus, Dendrobates minutus* and *Dendrobates pumilio* (Dendrobatidae). m/e 203(1), 202(2), 138(100). H_6-deriv., m/e 209, 138. Does not appear to form an *N*-Ac deriv.

Dihydro (?): **Dendrobates *Alkaloid 205***
$C_{14}H_{23}N$ 205.342
Trace alkaloid from skin extracts of *Dendrobates histrionicus* (Dendrobatidae). Tentative mol. formula. m/e 205(1), 204(2), 138(100).

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)
Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

Dendrobates Alkaloid 217 A-290

$C_{15}H_{23}N$ 217.353

Struct. unknown. A major alkaloid from skin extracts of one population of *Dendrobates bombetes* and *Dendrobates minutus*; minor constit. in *Dendrobates tricolor* (Dendrobatidae). m/e 217 (2), 216 (3), 152 ($C_{10}H_{18}N$, 100). H_6-deriv, m/e 223, 152. Did not form an *N*-Ac deriv.

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 225 A-291

$C_{14}H_{27}NO$ 225.373

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates tinctorius* (Dendrobatidae). Mol. formula tentative; m/e 225 (3), 224 (6), 208 (2), 168 (100), 152 (25). Possibly a hydroxypumiliotoxin C. Cannot be hydrogenated.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 233 A-292

$C_{16}H_{27}N$ 233.396

Struct. unknown. Minor alkaloid from skin extracts of *Dendrobates* sp. (Colombia) (Dendrobatidae). Mol. formula tentative; m/e 233 (2), 232 (2), 166 (100). Probably higher homologue of *Dendrobates* Alkaloid 223B, A-404 with 2 double bonds in the R side chain. H_4-deriv, m/e 237, 166.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 295 A-293

$C_{19}H_{37}NO$ 295.507

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates auratus* (Dendrobatidae). Mol. formula tentative; m/e 295 (3), 278 (4), 138 (100).

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 301 A-294

$C_{21}H_{35}N$ 301.514

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates azureus* (Dendrobatidae). Mol. formula tentative; m/e 301 (<1), 260 (100). Possibly a member of Pumiliotoxin-C class with an allyl R-substituent and a C_9H_{15} R′-substituent, see *Dendrobates* Alkaloid 167A, A-354.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 325 A-295

$C_{19}H_{35}NO_3$ 325.49

Struct. unknown. A major alkaloid from skin extracts of *Dendrobates fulguritus* and *Dendrobates minutus* (Dendrobatidae). Mol. formula tentative; m/e 325 (3), 308 (12), 280 (3), 210 (2), 182 (56), 114 (16), 112 (9), 70 (100). Forms H_2-deriv, m/e similar to H_4-deriv of Pumiliotoxin B.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-188 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 351 A-296

$C_{21}H_{37}NO_3$ 351.528

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates auratus* (Dendrobatidae). Mol. formula tentative; m/e 351 (6), 350 (2), 336 (4), 152 (38), 138 (65), 70 (100). Probably a member of the Pumiliotoxin A class, but the large peak at 138 is atypical.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Fritillaria Alkaloid 5 A-297

Fritillaria *Base 5*

Struct. unknown. Alkaloid from *Fritillaria raddeana* (Liliaceae), occurring with Raddeamine, R-7. Mp 245-247°.

Aslanov, Kh.A. *et al., Zh. Obshch. Khim.*, 1956, **26**, 579; *J. Gen. Chem. USSR (Engl. Transl.)*, 1956, **26**, 623

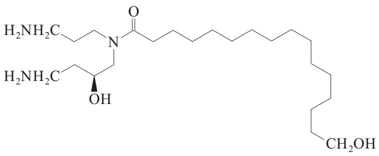
Fritillaria Alkaloid 6 A-298

Fritillaria *Base 6*

Struct. unknown. Alkaloid from *Fritillaria raddeana* (Liliaceae). Mp 197-199° (as hydrochloride).

Aslanov, Kh.A. *et al., Zh. Obshch. Khim.*, 1956, **26**, 579; *J. Gen. Chem. USSR (Engl. Transl.)*, 1956, **26**, 623

Fromia monilis Alkaloid A-299



$C_{23}H_{49}N_3O_3$ 415.658

***(S)*-form** [162340-03-6]

Alkaloid from the New Caledonian starfish *Fromia monilis*. Cytotoxic agent. $[\alpha]_D$ +3.5.

Palagiano, E. *et al., Tetrahedron*, 1995, **51**, 3675 (*isol, pmr, cmr, struct*)

Galanthus caucasicus Alkaloid A-300

$C_{17}H_{19}NO_4$ 301.341

Amaryllidaceae alkaloid. Struct. unknown. Isol. from *Galanthus caucasicus* (Amaryllidaceae). Cryst. (H_2O). Mp 214°. $[\alpha]_D^{20}$ +94.3 (c, 0.71 in MeOH).

Tsakadze, D.M. *et al., Khim. Prir. Soedin.*, 1969, **5**, 331; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 281 (*isol*)

Gentiana Alkaloid I A-301

$C_{13}H_{16}N_2O_3$ 248.281

Struct. unknown. Monoterpene alkaloid. Alkaloid from *Gentiana asclepiadea* and *Gentiana punctata* (Gentianaceae). Mp 183-187°.

Mollov, N.M. *et al., Dokl. Bulg. Akad. Nauk*, 1965, **18**, 947-949; *CA*, **64**, 10084h (*isol, uv, ir*)
Cordell, G.A. *et al., Alkaloids (Academic Press)*, 1977, **16**, 431 (*rev*)

Gentiana Alkaloid V A-302

$C_{10}H_9NO_2$ 175.187

Struct. unknown. Monoterpene alkaloid. Alkaloid from *Gentiana asclepiadea, Gentiana bulgarica, Gentiana cruciata, Gentiana lutea* (yellow gentian) and *Gentiana punctata* (Gentianaceae). Mp 240°.

Marekov, N. *et al., Dokl. Bulg. Akad. Nauk*, 1965, **18**, 999-1002; *CA*, **64**, 11270a (*isol, ir*)
Cordell, G.A. *et al., Alkaloids (Academic Press)*, 1977, **16**, 431 (*rev*)

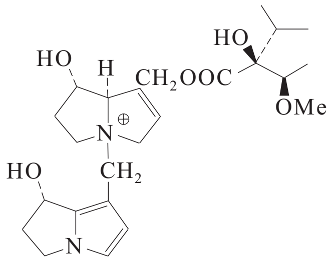
Gynura segetum Alkaloid A-303

$C_{18}H_{25}NO_5$ 335.399

Pyrrolizidine alkaloid. Struct. unknown. Possibly related to Seneciphylline, S-240. Alkaloid from *Gynura segetum*. Antimalarial agent. Cryst. Mp 223-224°.

Tang, S.-R. *et al., Zhongcaoyao*, 1980, **11**, 193-195; *CA*, **94**, 36187w

Heliotropium europaeum Alkaloid A-304



$C_{24}H_{37}N_2O_6^{\oplus}$ 449.566

Dimeric pyrrolizidine alkaloid, originally thought to be a C_{12} monomer. Alkaloid from *Heliotropium europaeum* (Boraginaceae). Prisms (Me_2CO/MeOH)(as chloride). Mp 158-159° dec. (as chloride). Results from alkylation of Heliotrine, H-95 by dehydroheliotrine in the plant. Does not appear to be an artifact.

Culvenor, C.C.J. *et al., Aust. J. Chem.*, 1954, **7**, 287 (*isol*)
Culvenor, C.C.J. *et al., Tet. Lett.*, 1969, 3603 (*pmr, struct*)

***Helleborus* Alkaloid V** A-305

$C_{25}H_{43}NO_6$ 453.618

Struct. unknown. Alkaloid from *Helleborus viridis.* Mp 267-268° (browns from 210°). V. weak base.

Keller, O. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1928, **266**, 545-572

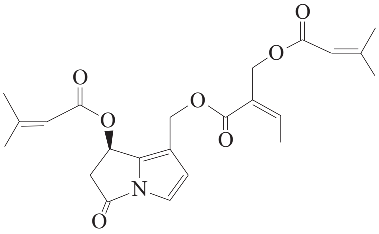
***Hovea longipes* Alkaloid** A-306

Struct. unknown. Alkaloid from the whole plant of *Hovea longipes* (Fabaceae). Cryst. (EtOH/HCl)(as hydrochloride). Mp 238-239° (hydrochloride).

Fitzgerald, J.S. *et al., An. Quim.*, 1972, **68**, 737 (*isol*)

***Jacmaia incana* Alkaloid** A-307

[78869-20-2]



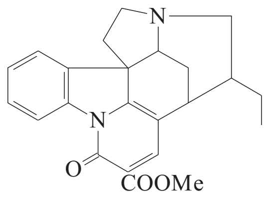
$C_{23}H_{27}NO_7$ 429.469

Alkaloid from the aerial parts of *Jacmaia incana* (Asteraceae). Gum. $[\alpha]_D^{24}$ -12 (c, 0.9 in $CHCl_3$). Closely related to the Senampelines (see Senampelines, S-233).

Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 831-832 (*ir, pmr, ms, struct*)

***Leuconotis* Alkaloid 376** A-308

[131242-30-3]



$C_{23}H_{24}N_2O_3$ 376.454

Alkaloid from *Leuconotis griffithii* and *Leuconotis eugenifolia.*

Goh, S.H. *et al., Tetrahedron*, 1989, **45**, 7899 (*isol, uv, ir, pmr, cmr, ms, struct*)

***Leuconotis griffithii* Alkaloid 308** A-309

Struct. and MF unknown. Alkaloid from *Leuconotis griffithii.*

Goh, S. *et al., Tetrahedron*, 1989, **45**, 7899-7820 (*isol, uv, pmr, cmr, ms*)

***Lycopodium* Alkaloid V** A-310

Lycopodium *Base V*

$C_{17}H_{27}NO_2$ 277.406

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae).

Methiodide: Mp 304°. $[\alpha]_D^{20}$ -66.

Methochloride: Mp 258°.

Methoperchlorate: Mp 321°.

Achmatowicz, O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1958, **32**, 485 (*isol, uv*)

***Lycopodium* Alkaloid X** A-311

Lycopodium *Base X*

$C_{17}H_{25}NO_3$ 291.389

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae).

Methiodide: Mp 315°. $[\alpha]_D^{18}$ -30.9.

Methochloride: Mp 269°.

Methoperchlorate: Mp 335°.

Methopicrate: Mp 151°.

Achmatowicz, O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1958, **32**, 485 (*isol, uv*)

***Lycopodium* Alkaloid 168** A-312

Lycopodium *Base 168*

$C_{16}H_{23}NO_3$ 277.363

Struct. unknown. Trace alkaloid from *Lycopodium clavatum* (Lycopodiaceae). Mp 168°.

Rodewald, W.J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1977, **51**, 1271 (*isol, ir, ms*)

***Lycopodium* Alkaloid 258** A-313

Lycopodium *Base 258*

Molecular formula not known; MW = 263. Struct. unknown. Trace alkaloid from *Lycopodium clavatum* (Lycopodiaceae). Mp 258°.

Rodewald, W.J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1977, **51**, 1271 (*isol*)

***Lycopodium annotinum* Alkaloid†** A-314

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae).

Perchlorate:

Cryst. (H_2O). Mp 234° dec.

Picrate: Mp 241-241.5° dec.

Methiodide:

Cryst. (EtOH). Mp 261° dec.

Bertho, A. *et al., Chem. Ber.*, 1952, **85**, 663 (*isol*)

***Lycopodium annotinum* Alkaloid†** A-315

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae).

Picrate:

Yellow rosettes (EtOH). Mp 121° dec. (sint. at 110°).

Methiodide:

Cryst. (EtOH). Mp 290°.

Bertho, A. *et al., Chem. Ber.*, 1952, **85**, 663 (*isol*)

***Lycopodium clavatum* Alkaloid** A-316

Struct. unknown. Alkaloid from *Lycopodium clavatum* var. *megastachyon* (Lycopodiaceae). Mp 261-263°.

Ayer, W.A. *et al., Can. J. Chem.*, 1962, **40**, 2088 (*isol*)

***Lycopodium thyoides* Alkaloid** A-317

$C_{18}H_{27}NO_3$ 305.416

Struct. unknown. Alkaloid from *Lycopodium thyoides* and *Lycopodium contiguum* (Lycopodiaceae).

Perchlorate:

Cryst. (Me_2CO). Mp 210-212°.

Ayer, W.A. *et al., Phytochemistry*, 1974, **13**, 653 (*isol, ir, ms*)

***Mantella* Alkaloid 161** A-318

$C_9H_{11}N_3$ 161.206

Struct. unknown. Trace alkaloid from skin extracts of the Madagascan frog *Mantella laevigata*. Minor alkaloid in *Mantella* sp. cf. *madagascariensis.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

***Mantella* Alkaloid 191** A-319

Struct. and MF unknown. Possibly related to Precoccinelline. Trace alkaloid from skin extracts of the Madagascan frog *Mantella betsileo.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ms*)

***Mantella* Alkaloid 317** A-320

Homopumiliotoxin 317

Struct. and MF unknown. Trace alkaloid from skin extracts of the Madagascan frog *Mantella betsileo.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ms*)

***Mucuna pruriens* Alkaloid X** A-321

Mucuna pruriens *Base X*

$C_{11}H_{25}NO_3$ 219.323

Struct. unknown. Alkaloid from *Mucuna pruriens* (Fabaceae). Mp 94-95°.

Picrate: Mp 130-132°.

Rakhit, S. *et al., Indian J. Pharm.*, 1956, **18**, 285; *CA*, **52**, 5748e (*isol*)

***Pachysandra* Alkaloid V** A-322

Pachysandra *Base V*

Steroidal alkaloid. Struct. unknown. Isol. from *Pachysandra terminalis* (Buxaceae). Mp 218-221°.

Kikuchi, T. *et al., Tet. Lett.*, 1964, 1817

Kikuchi, T. *et al., Yakugaku Zasshi*, 1967, **87**, 215; *CA*, **67**, 32888v

***Pancratium* Alkaloid 6** A-323

Pancratium *Base 6*

$C_{16}H_{17}NO_4$ 287.315

Amaryllidaceae alkaloid. Struct. unknown. Isol. from *Pancratium maritimum* (Amaryllidaceae). Needles (MeOH). Mp 267-270°. $[\alpha]_D^{21}$ -184 (c, 1.04 in MeOH).

Sandberg, F. *et al., J. Nat. Prod.*, 1963, **26**, 78-90 (*isol, ir*)

***Pancratium* Alkaloid 31** A-324

Pancratium *Base 31*

$C_{18}H_{21}NO_5$ 331.368

Amaryllidaceae alkaloid. Struct. unknown. Isol. from *Pancratium maritimum* (Amaryllidaceae). Prisms (Me_2CO). Mp 213-216° dec. $[\alpha]_D^{21}$ -61 (c, 1.23 in $CHCl_3$).

Sandberg, F. *et al., J. Nat. Prod.*, 1963, **26**, 78-90 (*isol, ir*)

Pancratium sickenbergi Alkaloid A-325

$C_9H_{13}NO_3$ 183.207

Amaryllidaceae alkaloid. Struct. unknown. Isol. from *Pancratium sickenbergeri* (Amaryllidaceae). Mp 161° dec.

Fahmy, I.R. *et al., J. Pharm. Sci. U.A.R.*, 1960, **1**, 133-147; *CA*, **56**, 10280i (*isol*)

Papaver rhoeas Alkaloid A-326

$C_{19}H_{19}NO_6$ 357.362

Struct. unknown. Alkaloid from *Papaver rhoeas.* Cryst. ($CHCl_3$/EtOH). Mp 208-209°. $[\alpha]_D^{23}$ +235 ($CHCl_3$).

Slavik, J. *et al., Chem. Listy*, 1958, **52**, 1957-1964; *CA*, **53**, 1640h (*isol*)

Pseudaxinyssa Alkaloid A-327

$C_9H_{14}BrN_5O$ 288.146

Struct. unknown. Isol. from the marine sponge *Pseudaxinyssa cantharella*. Amorph. $[\alpha]_D$ +15.

De Nanteuil, G. *et al., Tetrahedron*, 1985, **41**, 6019-6033

Rhynchosia pyramidalis Alkaloid A-328

Struct. unknown. Alkaloid from *Rhynchosia pyramidalis* (Fabaceae). Mp 132° (as picrate).

Ristic, S. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1962, **295**, 510; *CA*, **57**, 14180e

Rosmarinus officinalis Alkaloid 2 A-329

$C_{20}H_{27}NO_4$ 345.438

Struct. unknown. Isol. from rosemary (*Rosmarinus officinalis*) using NH_3 during extraction. Cryst. (toluene). Mp 197-198° dec. $[\alpha]_D$ +36 (c, 1.48 in dioxan). Artifact.

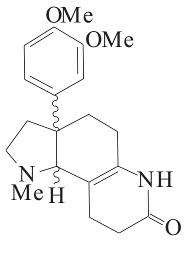
Hydrochloride:
Cryst. (H_2O). Mp 214-216° dec.

N,O,O-*Tri-Ac:*
Cryst. (MeOH). Mp 291-292° dec.

Yakhontova, L.D. *et al., Khim. Prir. Soedin.*, 1967, **3**, 140; *Chem. Nat. Compd. (Engl. Transl.)*, 1967, **3**, 118

Sceletium namaquense Alkaloid A-330

[82545-08-2]



$C_{20}H_{26}N_2O_3$ 342.437

Compd. not named in reference. Alkaloid from *Sceletium namaquense* (Aïzoaceae). Oil. Related to *Sceletium* Alkaloid A_4, A-346.

Jeffs, P.W. *et al., J.O.C.*, 1982, **47**, 3611 (*isol, ir, cd, pmr, ms, struct*)

Senecio borysthenicus Alkaloid A-331

$C_{18}H_{23}NO_5$ 333.383

Struct. unknown. Pyrrolizidine alkaloid. Alkaloid from *Senecio borysthenicus* (Asteraceae). Mp 195° dec. Conts. an OH group.

Red'ko, A.L. *et al., CA*, 1959, **53**, 20695

Senecio renardi Alkaloid 4 A-332

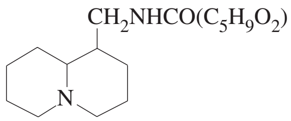
Senecio renardi *Base 4*

Struct. unknown. Alkaloid from *Senecio renardi* (Asteraceae). Cryst. (Me_2CO). Mp 176-178°.

Danilova, A.V. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1950, **20**, 1921; *CA*, **45**, 2960

Sophora Alkaloid 9 A-333

Sophora *Base 9*



$C_{16}H_{28}N_2O_3$ 296.409

Struct. of acyl group not known. Alkaloid from *Sophora alopecuroides* (Fabaceae). Related to Sophorine in O-59.

Kuchkarov, S. *et al., Khim. Prir. Soedin.*, 1979, **15**, 413-414; *Chem. Nat. Compd. (Engl. Transl.)*, 364-365

Strempeliopsis strempelioides Alkaloid A-334

Strempeliopsis *Bisindole base*

$C_{38}H_{46}N_4$ 558.808

Struct. unknown. Alkaloid from the roots of *Strempeliopsis strempelioides* (Apocynaceae). Mp 158-171°. $[\alpha]_D^{20}$ +210 ($CHCl_3$).

Laguna, A. *et al., Planta Med.*, 1984, **50**, 285-288 (*isol, uv, ir, ms*)

Thermopsis lanceolata Alkaloid A-335

Struct. unknown. Alkaloid from *Thermopsis lanceolata* epigeal parts (Fabaceae). Cryst. (Me_2CO). Mp 235°. $[\alpha]_D$ +121.8 (c, 1 in $CHCl_3$).

Vinogradova, V.I. *et al., Khim. Prir. Soedin.*, 1971, 463-466; *Chem. Nat. Compd. (Engl. Transl.)*, 440 (*isol*)

Ulex europaeus Alkaloid A-336

$C_{15}H_{20}N_2O_5$ 308.333

Struct. unknown. Alkaloid from shoots of *Ulex europaeus* (Fabaceae). Lustrous plates (petrol). Mp 170°.

Clemo, G.R. *et al., J.C.S.*, 1935, 10 (*isol*)

Uncaria callophylla Alkaloid A-337

Bisindole alkaloid; probably derived from Gambirine, G-13 and Pseudoyohimbine. Struct. unknown. Minor alkaloid from the leaves of *Uncaria callophylla* (Rubiaceae). Yellow powder. Mp 330°. Mol. formula not reported.

Goh, S.H. *et al., Phytochemistry*, 1985, **24**, 880-881 (*isol, uv, ir, pmr*)

Ungernia severtzovii Alkaloid A-338

$C_{17}H_{19}NO_3$ 285.342

Amaryllidaceae alkaloid. Struct. unknown. Isol. from the leaves of *Ungernia severtzovii* (Amaryllidaceae). Mp 186-187°. Opt. inactive.

Nitrate: Mp 245-246°.

Picrate: Mp 241-243°.

Smirnova, L.S. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **154**, 171-173; *CA*, **60**, 9324b (*isol*)

Veratrum Alkaloid X A-339

Steroidal alkaloid. Struct. unknown. Isol. from *Veratrum lobelianum* (Liliaceae). Needles (MeOH). Mp 215-217°. ir shows C═C, OH and NH_2 groups.

Shinkarenko, A.L. *et al., Khim. Prir. Soedin.*, 1966, **2**, 293; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 239

Voacanga thouarsii Alkaloid I A-340

[50924-03-3]

$C_{43}H_{48}N_4O_6$ 716.875

Bisindole alkaloid. Struct. unknown. Alkaloid from the leaves of *Voacanga thouarsii* (Apocynaceae). Amorph. Intense blue col. with HNO_3. λ_{max} 223 ; 264 ; 300 ; 327 (EtOH).

Rolland, Y. *et al., Phytochemistry*, 1973, **12**, 2039-2042 (*isol, uv, ir, pmr*)

Zephyranthes Alkaloid A-341

Amaryllidaceae alkaloid. Struct. unknown. Isol. from the bulbs of *Zephyranthes robusta* and *Zephyranthes sulphurea* (Amaryllidaceae). Stout prisms (MeOH). Mp 252-254°.

Rao, R.V.K. *et al., Indian J. Pharm.*, 1969, **31**, 62-63; 86-87; *CA*, **71**, 109780w; 128623p (*isol*)

Alkaloid 1 (Calabash curare) A-342

$C_{20}H_{21}N_2^{\oplus}$ 289.399

Struct. unknown. Alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). Mp 239-243° (as chloride). $[\alpha]_D^{20}$ -134 (c, 8.95 in H_2O) (chloride). Deep-blue col. with $Ce(SO_4)_2$.

Wieland, T. *et al., Chem. Ber.*, 1952, **85**, 731-743

Alkaloid 2 (Calabash curare) A-343

Struct. unknown. Quaternary alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). $[\alpha]_D^{20}$ -659 (as chloride). Red-violet col. with $Ce(SO_4)_2$.

► Toxic.

Wieland, T. *et al., Chem. Ber.*, 1952, **85**, 731

Lycopodium Alkaloid IV A-344

Lycopodium *Base IV*

$C_{16}H_{23}NO$ 245.364

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae).

Methiodide: Mp 265°. $[\alpha]^{20}_{D}$ -150.1.

Methochloride: Mp 210°.

Methoperchlorate: Mp 270°.

Methopicrate: Mp 230-232°.

Achmatowicz, O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1958, **32**, 485-498 (*isol, uv*)

Daphniphyllum Alkaloid A_1 A-345

$C_{23}H_{33}NO_3$ 371.519

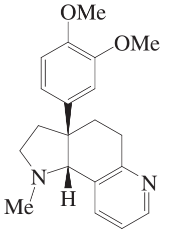
Struct. unknown. Alkaloid from the bark and leaves of *Daphniphyllum macropodum* (Daphniphyllaceae). Mp 225-226° (as methiodide).

Toda, M. *et al., Tetrahedron*, 1972, **28**, 1477 (*isol, ir, pmr, ms*)

Sceletium Alkaloid A_4 A-346

3a-*(3,4-Dimethoxyphenyl)-2,3,3*a,*4,5,9*b-*hexahydro-1-methyl-1*H-*pyrrolo[2,3-f]quinoline, 9CI*

[35135-35-4]



Absolute Configuration

$C_{20}H_{24}N_2O_2$ 324.422

Alkaloid from *Sceletium namaquense* and *Sceletium tortuosum* (Aïzoaceae). Prisms (EtOAc). Mp 153.3-154.5°. $[\alpha]_D$ +131 (MeOH).

Luhan, P.A. *et al., J.C.S. Perkin 2*, 1972, 2006 (*cryst struct*)

Jeffs, P.W. *et al., J.O.C.*, 1974, **39**, 2703 (*isol, uv, ir, pmr, ms, cd, struct*)

Martin, N.H. *et al., Org. Mass Spectrom.*, 1976, **11**, 1 (*ms*)

Stevens, R.V. *et al., Acc. Chem. Res.*, 1977, **10**, 193 (*synth*)

Kamikubo, T. *et al., Chem. Comm.*, 1998, 783-784 (*synth, abs config*)

Yamada, O. *et al., Tet. Lett.*, 1998, **39**, 7747-7750 (*synth*)

Hayashi, M. *et al., Tet. Lett.*, 2002, **43**, 1461-1464 (*synth*)

Abrus precatorius Alkaloid A A-347

Struct. unknown. Alkaloid from seeds of *Abrus precatorius.* Mp 143° dec.

Tung, Y.-C. *et al., CA*, 1960, **55**, 17770g; **61**, 9777c; *Biol. Abstr.*, **36**, 65720

Buxus Alkaloid A1 A-348

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *rotundifolia* (Buxaceae). Cryst. (CH_2Cl_2). Mp 195-197°. Contains NMe_2 group at C-3.

Huong, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1425-1432 (*isol, ms*)

Buxus Alkaloid A2 A-349

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *rotundifolia* (Buxaceae). Cryst. (Me_2CO/MeOH). Mp 138-142°.

Huong, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1425-1432 (*isol, ms*)

Buxus Alkaloid A3 A-350

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *rotundifolia* (Buxaceae). Cryst. (Me_2CO/MeOH). Mp 272-274°. $[\alpha]^{22}_{D}$ +20 (c, 0.25 in EtOH).

Huong, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1425-1432 (*isol, ms*)

Buxus Alkaloid A4 A-351

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *rotundifolia* (Buxaceae). Cryst. (CH_2Cl_2). Mp 252-256°. $[\alpha]^{22}_{D}$ -109 (c, 0.51 in MeOH).

Huong, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1425-1432 (*isol, ms*)

Buxus Alkaloid A5 A-352

$C_{40}H_{60}N_2O_7$ 680.923

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *rotundifolia* (Buxaceae). Cryst. (CH_2Cl_2). Mp 125-127°. $[\alpha]^{22}_{D}$ -10 (c, 0.3 in CH_2Cl_2).

Huong, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1425-1432 (*isol, ms*)

Chondrodendron limaciifolium Alkaloid A A-353

$C_{36}H_{38}N_2O_6$ 594.706

Struct. unknown. Bisbenzylisoquinoline alkaloid. Alkaloid from the wood of *Chondrodendron limaciifolium* (Menispermaceae). Thin plates or flattened needles (Py, $CHCl_3$/MeOH or MeOH). Mp 270-300° dec.

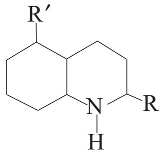
Sulfate:

Rhombic plates +$10H_2O$. Mp 289° (efferv.).

Barltrop, J.A. *et al., J.C.S.*, 1954, 159 (*isol*)

Dendrobates Alkaloid 167A A-354

2-Ethyldecahydroquinoline



$R = CH_2CH_3, \quad R' = H$

$C_{11}H_{21}N$ 167.294

Tentative struct. Trace alkaloid from skin extracts of *Dendrobates auratus* (Dendrobatidae). Mol. formula tentative; m/e 167(1), 166(1), 138(100). Cannot be hydrogenated.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

Dendrobates Alkaloid 181A A-355

2-Ethyldecahydro-5-methylquinoline

As *Dendrobates* Alkaloid 167A, A-354 with

$R = CH_2CH_3$, $R' = CH_3$

$C_{12}H_{23}N$ 181.32

Tentative struct. Trace alkaloid from skin extracts of *Dendrobates auratus* (Dendrobatidae). Mol. formula tentative; m/e 181(2), 180(1), 152(100). Cannot be hydrogenated.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

Dendrobates Alkaloid 209A A-356

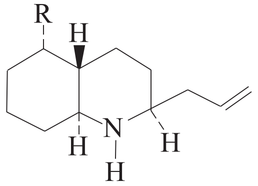
$C_{13}H_{25}NO$ 211.347

Struct. unknown. Trace alkaloid from skin extracts of an undescribed *Dendrobates* sp. from Panama (Dendrobatidae). Mol. formula tentative; m/e 209 (5), 168 (100). H_2-deriv, m/e 211, 168.

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 219A A-357

Decahydro-2,5-bis(2-propenyl)quinoline.
2,5-Diallyldecahydroquinoline



$R = CH_2CH = CH_2$

$C_{15}H_{25}N$ 219.369

A major constit. in skin extracts of *Dendrobates auratus, Dendrobates azureus, Dendrobates granuliferus, Dendrobates histrionicus, Dendrobates parvulus* and *Dendrobates truncatus* (Dendrobatidae). $[\alpha]^{24}_{D}$ +9.7 (c, 2.0 in MeOH).

Tetrahydro: Decahydro-2,5-dipropylquinoline. **Dendrobates** ***Alkaloid 223A***†. *Pumiliotoxin* C_{II}

[63983-61-9]

[112791-03-4 , 112790-00-8 , 112789-97-6 , 67920-43-8 , 112789-98-7]

$C_{15}H_{29}N$ 223.401

Minor or trace alkaloids in skin extracts of *Dendrobates auratus, Dendrobates histrionicus* (various populations), *Dendrobates lehmanni, Dendrobates minutus, Dendrobates occultator, Dendrobates truncatus* and *Dendrobates* sp. of Colombia (Dendrobatidae).

5-Epimer: **Dendrobates** ***Alkaloid 219A′***

$C_{15}H_{25}N$ 219.369

Present in skin extracts from one population of *Dendrobates histrionicus* and *Dendrobates auratus* (Dendrobatidae). $[\alpha]_D$ +5.8 (c, 0.31 in $CHCl_3$).

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)
Tokuyama, T. *et al., Tetrahedron*, 1986, **42**, 3453; 1991, **47**, 5401 (*isol, pmr, cmr, ms, cryst struct, abs config*)
McCloskey, P.J. *et al., J.O.C.*, 1988, **53**, 1380 (*tetrahydro, synth*)
Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)
Toyooka, N. *et al., J.O.C.*, 2002, **67**, 6078-6081 (*synth*)

***Dendrobates* Alkaloid 231A A-358**

5-Ethyldecahydro-2-(2-penten-4-ynyl)quinoline

As *Dendrobates* Alkaloid 167A, A-354 with
$R = -CH_2CH{=}CHC{\equiv}CH$,
$R' = CH_2CH_3$

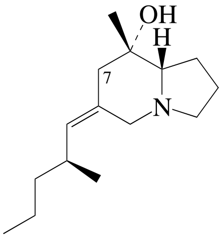
$C_{16}H_{25}N$ 231.38

Tentative struct. Minor alkaloid from skin extracts of *Dendrobates histrionicus* and *Dendrobates minutus* (Dendrobatidae). Mol. formula tentative; m/e 231(2), 230(1), 166(100). Forms H_6-deriv., m/e 237, 166. Does not appear to form an *N*-Ac deriv.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)
Spande, T.F. *et al., Phytochemistry*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

***Dendrobates* Alkaloid 237A A-359**

Octahydro-8-methyl-6-(2-methylpentylidene)-8-indolizinol, 9CI. 8-Hydroxy-8-methyl-6-(2-methylpentylidene)indolizidine
[73376-36-0]



$C_{15}H_{27}NO$ 237.384

Proposed struct. A major alkaloid from skin extracts of *Dendrobates abditus*; trace constit. in *Dendrobates histrionicus* (Dendrobatidae).

7-Hydroxy: **Dendrobates *Alkaloid 253A***
[73376-37-1]
$C_{15}H_{27}NO_2$ 253.384
A major alkaloid of *Dendrobates abditus*; minor constit. in *Dendrobates lehmanni* and *Dendrobates auratus* (Dendrobatidae). Stereochem. undefined.

7-Hydroxy, didehydro (?): **Dendrobates *Alkaloid 251E***
$C_{15}H_{25}NO_2$ 251.368
Minor alkaloid from skin extracts of *Dendrobates minutus* (Dendrobatidae). Mol. formula and structure tentative; m/e 251(3), 250(1), 234(2), 168(30), 84(18), 70(100).

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)
Daly, J.W. *et al., J.A.C.S.*, 1980, **102**, 830 (*struct*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)
Thanh, G.V. *et al., Tet. Lett.*, 1999, **40**, 3713-3716 (*synth*)

***Dendrobates* Alkaloid 239A A-360**

$C_{15}H_{29}NO$ 239.4

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates occultator* (Dendrobatidae). Mol. formula tentative; m/e 239 (2), 238 (3), 182 (100). Cannot be hydrogenated.

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

***Dendrobates* Alkaloid 241A A-361**

Dendrobates *Alkaloid 241*
Struct. unknown
Trace alkaloid from skin extracts of *Dendrobates occultator* (Dendrobatidae). Mol. formula not known; m/e 241 (2), 240 (3), 166 (100), 126 (48). Does not separate from major alkaloids 239 *A, B, C, D.*

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

***Dendrobates* Alkaloid 243A A-362**

Decahydro-5-(2-penten-4-ynyl)-2-(2-propenyl)quinoline. 2-Allyl-5-(2-penten-4-ynyl)decahydroquinoline

As *Dendrobates* Alkaloid 219A, A-357 with
$R = -CH_2CH{=}CHC{\equiv}CH$ (*Z*-)

$C_{17}H_{25}N$ 243.391

A major alkaloid in *Dendrobates auratus, Dendrobates azureus, Dendrobates granuliferus, Dendrobates histrionicus*; minor or trace constit. in *Dendrobates pictus, Dendrobates tinctorius, Dendrobates trivittatus* and *Dendrobates truncatus* (Dendrobatidae). $[\alpha]_D^{16}$ -15.2 (c, 1.37 in MeOH). $[\alpha]_D^{16}$ -30.7 (c, 1.37 in $CHCl_3$).

Stereoisomer: Dendrobates *Alkaloid 243A′*
$C_{17}H_{25}N$ 243.391
Present in some skin extracts of *Dendrobates* spp. (Dendrobatidae). $[\alpha]_D^{16}$ -0.96 (c, 0.73 in MeOH). $[\alpha]_D^{16}$ -18.6 (c, 0.73 in $CHCl_3$). Of unknown config.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)
Tokuyama, T. *et al., Tetrahedron*, 1986, **42**, 3453 (*isol, pmr, cmr, struct*)
Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

***Dendrobates* Alkaloid 251A A-363**

$C_{17}H_{33}N$ 251.454

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates histrionicus* (Dendrobatidae). Mol. formula tentative; m/e 251 (2), 208 (6), 152 (100). Possibly in Pumiliotoxin-C class with R = C_7H_{15} (see *Dendrobates* Alkaloid 223C, A-438 and *Dendrobates* Alkaloid 167A, A-354.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

***Dendrobates* Alkaloid 257A A-364**

$C_{18}H_{25}N$ 255.402

Struct. unknown. Minor alkaloid from skin extracts of *Dendrobates trivittatus* (Dendrobatidae). Mol. formula tentative; m/e 257 (1), 256 (2), 216 (100). Cannot be acetylated, but consumes 4 molar equivs. of H_2. Possibly a perhydropyrroloquinoline of the gephyrotoxin class.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

***Dendrobates* Alkaloid 265A A-365**

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates abditus, Dendrobates auratus, Dendrobates azureus, Dendrobates histrionicus, Dendrobates lehmanni, Dendrobates occultator, Dendrobates parvulus* and *Dendrobates tinctorius* (Dendrobatidae). Mol. formula not known; m/e 265 (50), 264 (100), 222 (58), 180 (72). Very atypical mass spectrum for a dendrobatid alkaloid. Possibly a degradation artifact.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

***Dendrobates* Alkaloid 269A A-366**

Decahydro-2-(3,4-pentadienyl)-5-(2-penten-4-ynyl)quinoline, 9CI. Dendrobates histrionicus *Alkaloid III*
[63983-62-0]

As *Dendrobates* Alkaloid 167A, A-354 with
$R = CH_2CH_2CH{=}C{=}CH_2$,
$R' = CH_2CH{=}CHCdCH$

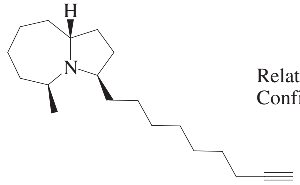
$C_{19}H_{27}N$ 269.429

Tentative struct. Minor or trace alkaloid in skin extracts of *Dendrobates granuliferus, Dendrobates histrionicus* (several populations), *Dendrobates occultator, Dendrobates trivittatus* and *Dendrobates truncatus* (Dendrobatidae), also in skin of the Madagascan frog *Mantella madagascariensis* (Ranidae, subfamily Mantellinae). m/e 269(4), 268(12), 204(100). H_{10}-deriv., m/e 279, 208.

Daly, J.W. *et al., Helv. Chim. Acta*, 1977, **60**, 1128 (*isol, ms*)
Daly, J.W. *et al., Toxicon*, 1978, **16**, 163; 1984, **22**, 905 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)
Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

Dendrobates Alkaloid 275A A-367

Octahydro-5-methyl-10-(8-nonynyl)-1H-pyrrolo[1,2-a]azepine, 9CI. 5-Methyl-10-(8-nonynyl)lehmizidine



Relative Configuration

$C_{19}H_{33}N$ 275.476

Major alkaloid from the skin extracts of the frog *Dendrobates lehmanni*.

8,9-Dihydro: Octahydro-5-methyl-10-(8-nonenyl)-1H-pyrrolo[1,2-a]azepine. **Dendrobates *Alkaloid 277A***. *5-Methyl-10-(8-nonenyl)lehmizidine*
$C_{19}H_{35}N$ 277.492
Alkaloid from *Dendrobates lehmanni*.

Oxo: Octahydro-5-methyl-10-(oxo-8-nonynyl)-1H-pyrrolo[1,2-a]azepine. **Dendrobates *Alkaloid 289A***
$C_{19}H_{31}NO$ 289.46
Alkaloid from *Dendrobates lehmanni*. Posn. of oxo group not known.

6′,7′-Didehydro, 8,9-dihydro: Octahydro-5-methyl-10-(6,8-nonadienyl)-1H-pyrrolo[1,2-a]azepine. **Dendrobates *Alkaloid 275G***. *5-Methyl-10-(6,8-nonadienyl)lehmizidine*
$C_{19}H_{33}N$ 275.476
Alkaloid from *Dendrobates lehmanni*. Tentative struct. assigned.

3,5-Diepimer: **Dendrobates *Alkaloid 275A′***
$C_{19}H_{33}N$ 275.476
Alkaloid from *Dendrobates lehmanni*.

[120037-67-4]

Garraffo, H.M. *et al., J. Nat. Prod.*, 2001, **64**, 421-427

Dendrobates Alkaloid 281A A-368

$C_{17}H_{31}NO_2$ 281.437

Struct. unknown. A major alkaloid from skin extracts of *Dendrobates minutus*; trace constit. in *Dendrobates abditus.* Mol. formula tentative; m/e 281(4), 280(2), 264(2), 194(12), 166(72), 70(100). H_2-deriv., m/e 283(1), 282(2), 266(4), 208(40), 138(10), 110(10), 84(100), 70(85).

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-188 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 297A A-369

$C_{17}H_{31}NO_3$ 297.437

Struct. unknown. A major alkaloid from skin extracts of *Dendrobates minutus* (Dendrobatidae). m/e 297 (3), 296 (4), 280 (9), 236 (2), 210 (3), 194 (4), 193 (3), 182 (21), 114 (27), 112 (16), 70 (100). Lowest molecular-weight member of the Pumiliotoxin-A class to contain 3 oxygens. H_2-deriv, m/e 299 (4), 282 (12), 256 (6), 224 (4), 110 (50), 84 (100), 70 (75).

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 309A A-370

Dihydropumiliotoxin A

$C_{19}H_{35}NO_2$ 309.491

Struct. unknown. Minor alkaloid from skin extracts of *Dendrobates minutus* and *Dendrobates viridis* (Dendrobatidae). Mol. formula tentative; m/e 309 (9), 308 (3), 292 (2), 280 (4), 206 (4), 194 (15), 176 (5), 166(100), 110 (10), 84 (20), 70 (51). Forms H_2-deriv.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-188 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Erythrophleum Alkaloid A A-371

$C_{25}H_{37}NO_6$ 447.57

Struct. unknown. Dimethylaminoethanol esterified with an α,β-unsaturated diterpene acid carrying a methoxycarbonyl group and 3 Me groups. UV shows no evidence for a 6,7-dione as observed in other *E.* alkaloids. Alkaloid from the bark of *Erythrophleum africanum* (Fabaceae). Cryst. (Et_2O/hexane). Mp 105°. Poss. identical with an alkaloid from *E. guineense* with the same MF. No further data to 2007.

Friedrich-Fichtl, J. *et al., Chem. Ber.*, 1971, **104**, 3535-3548 (*Erythrophleum guineense alkaloid*)
Jansson, S. *et al., Acta Pharm. Suec.*, 1976, **13**, 51-54; *CA*, **84**, 147726j (*isol, uv, ir, pmr, ms*)

Euonymus Alkaloid A A-372

$C_{29}H_{37}NO_{13}$ 607.61

Struct. unknown. Alkaloid from the seeds of *Euonymus europaea*. Mp 258-260°. $[\alpha]_D$ +21 ($CHCl_3$).

De-Ac: **Euonymus *Alkaloid B***
$C_{27}H_{35}NO_{12}$ 565.573
Alkaloid from the seeds of *Euonymus europaea*. Mp 288-290°. $[\alpha]_D$ +14 ($CHCl_3$).

Ac: **Euonymus *Alkaloid C***
$C_{31}H_{39}NO_{14}$ 649.647
Alkaloid from the seeds of *Euonymus europaea*. Mp 164-168°. $[\alpha]_D$ +8 ($CHCl_3$).

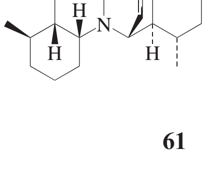
Doebel, K. *et al., Helv. Chim. Acta*, 1949, **32**, 592-597 (*isol*)

Fritillaria Alkaloid A A-373

Struct. unknown. Alkaloid from *Fritillaria meleagris* (Liliaceae). Mp 156-158°. Cooccurs with Imperialine in C-298.

Bauer, S. *et al., Chem. Zvesti*, 1958, **12**, 584

Mantella Alkaloid 384A A-374



Relative Configuration

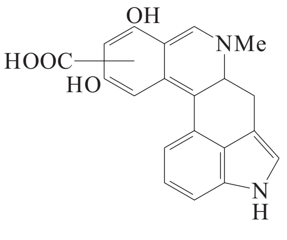
$C_{26}H_{44}N_2$ 384.647

Tentative struct. shown. Obt. as mixt. with *Mantella* Alkaloid 384B. Major constit. of skin extracts of the Madagascan frog *Mantella betsileo*. Minor constit. in *Mantella* sp. cf. *madagascariensis* and *Mantella laevigata*. No CAS no. found to 15CI.

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

Securidaca longipedunculata Alkaloid A A-375

[146442-66-2]



$C_{20}H_{16}N_2O_4$ 348.357

Alkaloid from roots of *Securidaca longipedunculata* (Polygalaceae).

Costa, C. *et al., J. Het. Chem.*, 1992, **29**, 1641-1647

Stephania glabra Alkaloid A A-376

Stephania glabra *Base A*

$C_{19}H_{21}NO_4$ 327.379

Struct. unknown, conts. 2 OMe groups. Authors suggest the struct. to be *N*-methylhydroxystepharine. Isol. from herbage of *Stephania glabra*. Mp 205-206°. $[\alpha]_D^{21}$ -70. λ_{max} 242 ; 282 (no solvent reported).

Shchelchkova, I.I. *et al., Khim. Prir. Soedin.*, 1965, **1**, 271-275; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 210-212 (*isol*)

Stephania glabra Alkaloid A A-377

$C_{19}H_{18}NO_2$ 292.357

Struct. unknown. The MF assigned is impossible. Isol. from tubers of *Stephania glabra*. Cryst. (Et_2O). Mp 79-81°. $[\alpha]_D$ -88 (c, 1 in EtOH). Prob. an aporphine alkaloid. Contains an NMe group. No further reports, although later investigations of the species have been reported.

Hydrochloride: Mp 252-253°.

N-*Ac:*
Cryst. (Me_2CO). Mp 146°.

Kin, F.K. *et al., Khim. Prir. Soedin.*, 1965, **1**, 392-394; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 308-309 (*isol*)
Cava, M.P. *et al., J.O.C.*, 1968, **33**, 2785-2789 (*Stephania glabra constits*)

Stephania japonica Alkaloid A A-378

Stephania *Base A*

$C_{21}H_{26}ClNO_7$ 439.892

Struct. unknown. Alkaloid from the stems and rhizomes of *Stephania japonica* var. *australis* (Menispermaceae). Prisms (MeOH). Mp 248°. Ir shows OH and γ-lactam groups, pmr shows 4 OMe groups, 1 NMe group, and 2 aromatic protons. Ms m/e 257.1068, indicating a hasubanan alkaloid.

Matsui, M. *et al., Phytochemistry*, 1979, **18**, 1087 (*isol, ir, pmr, ms*)

Taxus baccata Alkaloid A A-379

$C_{33}H_{43}N_2O_{14}$ 691.708

Struct. unknown. The MF given is impossible. Isol. from leaves of *Taxus baccata*. Cryst. (petrol). Mp 112-113°. $[\alpha]_D^{17}$ +10.7 (c, 0.835 in $CHCl_3$). Co-occurs with Taxol, T-52.

Mirzoev, Kh.M. *et al., Khim. Prir. Soedin.*, 1970, **6**, 777-778; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 797

Thermopsis lanceolata Alkaloid A A-380

[78040-76-3]

Struct. unknown. Constit. of *Thermopsis lanceolata*.

Chao, K.-S. *et al., CA*, 1981, **95**, 35461q (*isol, props*)

Alangium Alkaloid AL64 A-381

$C_{29}H_{37}N_3O_3$ 475.63

Struct. unknown. Poss. identical with Alangimarckine in T-675. Alkaloid from the root bark of *Alangium lamarckii* (Alangiaceae). Glistening needles (CH_2Cl_2 and/or MeOH). Mp 272°. $[\alpha]_D$ -64 ($CHCl_3$). λ_{max} 226 (log ε 4.28); 283 (log ε 4.18) (EtOH).

Mono-Ac: Mp 184°.

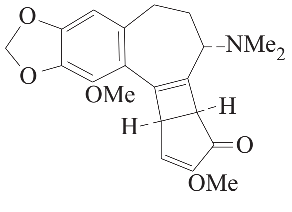
Di-Ac: Mp 150°.

Pakrashi, S. *et al., Indian J. Chem.*, 1964, **2**, 468 (*isol, uv*)

Alkaloid AM 3 A-382

N-*Deacetyl*-N,N-*dimethyl*-γ-*lumicornigerine*

[99499-80-6]



$C_{21}H_{23}NO_5$ 369.416

Alkaloid from the aerial parts of *Androcymbium melanthioides* var. *stricta* (Liliaceae). Needles. Mp 245-247°. $[\alpha]_D^{23}$ -391 (c, 1.0 in $CHCl_3$).

Potěšilová, H. *et al., Planta Med.*, 1985, 344 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

Alangium Alkaloid B1 A-383

$C_{20}H_{31}NO_5$ 365.469

Struct. unknown. Alkaloid from the bark of *Alangium lamarckii*. Mp 197-198° Mp 228-229° (as hydrochloride).

Basu, N.K. *et al., J. Indian Chem. Soc.*, 1957, **34**, 629-639; *CA*, **52**, 7337g

Alangium Alkaloid B2 A-384

$C_{27}H_{43}NO_6$ 477.64

Struct. unknown. Alkaloid from the bark of *Alangium lamarckii*. Mp 119-120° Mp 188° (as hydrochloride).

Basu, N.K. *et al., J. Indian Chem. Soc.*, 1957, **34**, 629-639; *CA*, **52**, 7337g

Alangium Alkaloid B3 A-385

Struct. unknown. Alkaloid from the bark of *Alangium lamarckii*. Mp 160-161° Mp 181° (as hydrochloride).

Basu, N.K. *et al., J. Indian Chem. Soc.*, 1957, **34**, 629-639; *CA*, **52**, 7337g

Alangium Alkaloid B4 A-386

$C_{19}H_{27}NO_7$ 381.425

Struct. unknown. Alkaloid from the bark of *Alangium lamarckii*. Mp 149-151° Mp 199° (as hydrochloride).

Basu, N.K. *et al., J. Indian Chem. Soc.*, 1957, **34**, 629-639; *CA*, **52**, 7337g

Alangium Alkaloid B5 A-387

$C_{21}H_{31}NO_8$ 425.478

Struct. unknown. Alkaloid from the bark of *Alangium lamarckii*. Mp 177-179° Mp 208° (as hydrochloride).

Basu, N.K. *et al., J. Indian Chem. Soc.*, 1957, **34**, 629-639; *CA*, **52**, 7337g

Asteracantha Alkaloid B1 A-388

Struct. unknown. Alkaloid from *Asteracantha longifolia* (preferred genus name *Hygrophila*). Mp 294°.

Basu, N.K. *et al., Indian J. Pharm.*, 1952, **14**, 212-213; *CA*, **47**, 4044g

Asteracantha Alkaloid B2 A-389

$C_5H_{13}NO_3$ 135.163

Struct. unknown. Alkaloid from *Asteracantha longifolia* (preferred genus name *Hygrophila*). Mp 194°.

Basu, N.K. *et al., Indian J. Pharm.*, 1952, **14**, 212-213; *CA*, **47**, 4044g

Buxus Alkaloid B A-390

$C_{24}H_{42}N_2O$ 374.609

Struct. unknown. Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 205-207°.

Schlittler, E. *et al., Helv. Chim. Acta*, 1949, **32**, 2209-2226 (*isol*)

Buxus Alkaloid B1 A-391

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *rotundifolia* (Buxaceae). Cryst. (Me_2CO/MeOH). Mp 280° dec. $[\alpha]_D^{22}$ +11.8 (c, 0.55 in MeOH). Contains MeNH group. λ_{max} 243 (log ε 4.19) (MeOH).

Huong, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1425-1432 (*isol, uv, ms*)

Buxus Alkaloid B4 A-392

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *rotundifolia* (Buxaceae). Cryst. ($CHCl_3$). Mp 150-152°.

Huong, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1425-1432 (*isol, ms*)

Buxus Alkaloid B5 A-393

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *rotundifolia* (Buxaceae). Cryst. ($CHCl_3$). Mp 179-182°. $[\alpha]_D^{22}$ +9.6 (c, 0.5 in $CHCl_3$).

Huong, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1425-1432 (*isol, ms*)

Buxus Alkaloid B6 A-394

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *rotundifolia* (Buxaceae). Cryst. (MeOH). Mp 214-216°. $[\alpha]_D^{22}$ +6.6 (c, 0.15 in MeOH). Contains OH group and C_6-C_7 double bond.

Huong, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1425-1432 (*isol, ir, ms*)

Buxus Alkaloid B7 A-395

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *rotundifolia* (Buxaceae). Cryst. (Me_2CO). Mp 245-247°.

Huong, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1425-1432 (*isol, ms*)

Buxus Alkaloid B8 A-396

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *rotundifolia* (Buxaceae). Cryst. (Me_2CO). Mp 265°. $[\alpha]_D^{22}$ +34.6 (c, 0.54 in $CHCl_3$). Mass spec. indicated a MeNH group at C-20 and a dimethyl group at C-3.

Huong, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1425-1432 (*isol, ms*)

Buxus Alkaloid B387 A-397

$C_{25}H_{41}NO_2$ 387.604

Steroidal alkaloid. Struct. unknown. Alkaloid from *Buxus microphylla* var. *sinica* (Buxaceae). Mp 188-189°. $[\alpha]_D$ +6.7 ($CHCl_3$). ORD spectrum resembles that of 4,4*a*-dihydrobuxpiine.

Bauerová, O. *et al., Pharmazie*, 1973, **28**, 212-214; *CA*, **78**, 156665s (*isol, ir, uv, ms, ord*)

Buxus Alkaloid B398 A-398

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *argentea* (Buxaceae). Cryst. (C_6H_6/MeOH). Mp 197-199°.

Kuchkova, K.I. *et al., Chem. Zvesti*, 1976, **30**, 174-178 (*isol*)

Buxus Alkaloid B426 A-399

Struct. unknown. Alkaloid from *Buxus sempervirens* var. *argentea* (Buxaceae). Cryst. (MeOH/CH_2Cl_2). Mp 208-210°.

Kuchkova, K.I. *et al., Chem. Zvesti*, 1976, **30**, 174-178; *CA*, **87**, 2362q (*isol*)

C-Alkaloid B A-400

$C_{20}H_{23}N_2O^{\oplus}$ 307.414

Minimum formula. Struct. unknown. Alkaloid from calabash curare and *Strychnos mitscherlichii* (Loganiaceae).

Mp 270° (as picrate). Red-violet col. with $Ce(SO_4)_2$, becoming brown on standing.

Schmid, H. *et al., Helv. Chim. Acta*, 1952, **35**, 1864-1879; 1953, **36**, 102-121

Dendrobates Alkaloid 181B **A-401**

Decahydro-2-propylquinoline

As *Dendrobates* Alkaloid 167A, A-354 with

$R = C_3H_7$, $R' = H$

$C_{12}H_{23}N$ 181.32

Tentative struct. Trace alkaloid from skin extracts of *Dendrobates auratus, Dendrobates azureus, Dendrobates fulguritus* and *Dendrobates trivittatus* (Dendrobatidae). Mol. formula tentative; m/e 181(2), 180(2), 138(100). Cannot be hydrogenated.

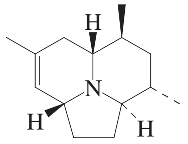
Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

Dendrobates Alkaloid 205B **A-402**

Alkaloid 205B



Absolute Configuration

$C_{14}H_{23}N$ 205.342

Proposed gross struct. confirmed and stereochem. revised in 2003. Trace alkaloid from skin extracts of the Panamanian poison-frog *Dendrobates pumilio* (Dendrobatidae). $[\alpha]_D$ -8.5 (c, 0.59 in $CHCl_3$).

Tokuyama, T. *et al., Tetrahedron*, 1987, **43**, 643 (*isol, pmr, cmr, ms, struct*)

Toyooka, N. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 3808-3810 (*synth, abs config*)

Smith, A.B. *et al., J.O.C.*, 2006, **71**, 2547-2557 (*synth*)

Dendrobates Alkaloid 219B **A-403**

Decahydro-5-methyl-2-(2,4-pentadienyl)-quinoline

As *Dendrobates* Alkaloid 167A, A-354 with

$R = -CH_2CH{=}CHCH{=}CH_2$,
$R' = CH_3$

$C_{15}H_{25}N$ 219.369

Tentative struct. Minor alkaloid from skin extracts of *Dendrobates histrionicus* and *Dendrobates* sp. (Colombia), trace constit. in *Dendrobates azureus* (Dendrobatidae). Mol. formula tentative, m/e 219(1), 218(2), 152(100). H_4-deriv., m/e 223, 152.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

Dendrobates Alkaloid 223B **A-404**

As *Dendrobates* Alkaloid 167A, A-354 with

$R = C_4H_9$, $R' = CH_2CH_3$

$C_{15}H_{29}N$ 223.401

Tentative struct. Minor or trace alkaloid in skin extracts of *Dendrobates auratus, Dendrobates histrionicus, Dendrobates minutus, Dendrobates truncatus* and *Dendrobates* sp. of Colombia (Dendrobatidae). m/e 223(1), 222(2), 166(100). Cannot be hydrogenated.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

Dendrobates Alkaloid 225B **A-405**

[103881-40-9]

$C_{15}H_{31}N$ 225.417

Struct. unknown. May be a 2,6-dipentylpiperidine. Trace constit. of *Dendrobates histrionicus* and a minor constit. in an undescribed *Dendrobates* sp. from Panama (Dendrobatidae).

Daly, J.W. *et al., J. Nat. Prod.*, 1986, **49**, 265-280

Dendrobates Alkaloid 231B **A-406**

As *Dendrobates* Alkaloid 167A, A-354 with

$R = C_6H_7$, $R' = CH_3$

$C_{16}H_{25}N$ 231.38

Tentative struct. Minor or trace alkaloid from skin extracts of *Dendrobates azureus, Dendrobates histrionicus, Dendrobates lehmanni, Dendrobates occultator, Dendrobates tinctorius* and *Dendrobates* sp. (Colombia) (Dendrobatidae). Mol. formula tentative; m/e 231(2), 230(1), 152(100). Forms H_6-deriv. m/e 237, 152.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

Dendrobates Alkaloid 237B **A-407**

$C_{14}H_{23}NO_2$ 237.341

Struct. unknown. Trace constit. in skin extracts of *Dendrobates abditus* and *Dendrobates fulguritus* (Dendrobatidae). Mol. formula tentative; m/e 237 (1), 236 (2), 182 (60), 114 (30), 112 (25), 70 (100).

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-188 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 239B **A-408**

$C_{15}H_{29}NO$ 239.4

Struct. unknown. Minor alkaloid from skin extracts of *Dendrobates bombetes*; trace constit. in *Dendrobates occultator* (Dendrobatidae). Mol. formula tentative; m/e 239 (2), 238 (3), 180 (100). Cannot be hydrogenated.

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 253B **A-409**

$C_{16}H_{33}NO$ 255.443

Struct. unknown. Trace alkaloid from skin extracts of an undescribed *Dendrobates* sp. from Panama (Dendrobatidae). Mol. formula tentative; m/e 253 (1), 138 (100). Cannot be hydrogenated.

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 257B **A-410**

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates lehmanni* (Dendrobatidae). Mol. formula not known; m/e 257 (60), 256 (100), 152 (20). Very atypical mass spectrum for a dendrobatid alkaloid. Possibly a degradation artifact.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 267B **A-411**

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates auratus* and *Dendrobates minutus* (Dendrobatidae). Mol. formula not known; m/e 267 (7), 266 (4), 250 (1), 170 (100), 152 (4), 112 (13). The base peak is atypical for a dendrobatid alkaloid.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 269B **A-412**

As *Dendrobates* Alkaloid 167A, A-354 with

$R = CH_2CH{=}CHC{\equiv}CH$,
$R' = CH_2CH{=}CHCH{=}CH_2$

$C_{19}H_{27}N$ 269.429

Tentative struct. Minor or trace alkaloid in skin extracts of *Dendrobates granuliferus, Dendrobates histrionicus* (several populations), *Dendrobates occultator, Dendrobates trivittatus* and *Dendrobates truncatus* (Dendrobatidae). m/e 269(4), 286(12), 202(100). H_{10}-deriv., m/e 279, 208.

Daly, J.W. *et al., Helv. Chim. Acta*, 1977, **60**, 1128 (*isol, ms*)

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 281B **A-413**

$C_{18}H_{35}NO$ 281.481

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates granuliferus* (Dendrobatidae). Mol. formula tentative; m/e 281 (4), 264 (12), 208 (25), 206 (20), 150 (65), 98 (5), 96 (20), 70 (100). Atypical spectrum for a dendrobatid alkaloid. Probably in

Pumiliotoxin-A class. Cannot be hydrogenated.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 283B A-414

$C_{17}H_{33}NO_2$ 283.453

Struct. unknown. A major alkaloid in skin extracts of *Dendrobates histrionicus* and *Dendrobates occultator* (Dendrobatidae). m/e 283 (<1), 282 (1), 254 (2), 212 ($C_{12}H_{22}NO_2$, 40), 152 ($C_{10}H_{18}N$, 23), 140 ($C_9H_{18}N$, 100). Cannot be hydrogenated.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 297B A-415

$C_{18}H_{35}NO_2$ 297.48

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates auratus* (Dendrobatidae). m/e 297 (10), 166 (92), 70 (100). Forms H_4-deriv.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-188 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 307B A-416

Isopumiliotoxin A
[67255-98-5]

$C_{19}H_{33}NO_2$ 307.475

Struct. unknown. Isomer of Pumiliotoxin A, P-791 without a large fragment ion for loss of OH. Minor or trace alkaloid in skin extracts of *Dendrobates auratus*, *Dendrobates granuliferus*, *Dendrobates lehmanni*, *Dendrobates minutus* and *Dendrobates pumilio* (Dendrobatidae). m/e 307 (12), 306 (4), 290 (2), 194 (24), 193(45), 166 (100), 70 (56). H_2-deriv, m/e 309(1), 280 (3), 208 (10), 138 (25), 110 (60), 84(100), 70 (45). H_4-deriv, m/e 311 (1), 110(25), 84 (100), 70 (30).

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-188 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 309B A-417

$C_{20}H_{39}NO$ 309.534

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates auratus* and *Dendrobates granuliferus* (Dendrobatidae). Mol. formula tentative; m/e 309 (1), 152 (100). Possibly member of Hydroxy pumiliotoxin-C class with OH group in the side chain.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Gentiana macrophylla Alkaloid B A-418

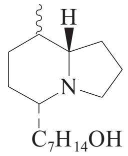
$C_9H_9NO_2$ 163.176

Struct. unknown. Monoterpene alkaloid. Alkaloid from the roots of *Gentiana macrophylla* (Gentianaceae). Cryst. (C_6H_6/petrol). Mp 128-130°.

Fu, F.-Y. *et al., Yaoxue Xuebao*, 1958, **6**, 198-203; *CA*, **53**, 8310b (*isol, uv*)

Mantella Alkaloid 253B A-419

(Octahydro-8-methyl-5-indolizinyl)-sec-heptanol, 9CI. *Indolizidine 253B*
[151871-22-6]



$C_{16}H_{31}NO$ 253.427

Provisional struct. Secondary alcohol. Minor alkaloid from skin extracts of one population of the Madagascan frog *Mantella madagascariensis.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016 (*isol, ir, ms*)

Mantella Alkaloid 271B A-420

Struct. and MF unknown. Trace alkaloid from skin extracts of the Madagascan frog *Mantella betsileo.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

Mantella Alkaloid 293B A-421

Struct. and MF unknown. Minor alkaloid from skin extracts of the Madagascan frog *Mantella* sp. cf. *madagascariensis.* Minor or trace constit. in *Mantella madagascariensis.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

Mantella Alkaloid 295B A-422

Struct. and MF unknown. Tentatively classified as an indolizidine. Forms a di-*O*-Ac deriv. Minor alkaloid from skin extracts of the Madagascan frog *Mantella crocea.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

Pseudophryne Alkaloid 252B A-423

$C_{14}H_{24}N_2O_2$ 252.356

Struct. unknown. Possibly analogous to Spiropyrrolizidine 252, S-437 but with the hydroxy group in another part of the struct. Minor alkaloid from skin extracts of one population of the Australian frog *Pseudophryne coriacea* (trace constit. in a different population of the same frog).

Daly, J.W. *et al., J. Nat. Prod.*, 1990, **53**, 407-421 (*isol, ms*)

Skytanthus acutus Alkaloid B A-424

$C_{11}H_{21}N$ 167.294

Struct. unknown. Monoterpene alkaloid. Alkaloid from *Skytanthus acutus* (Apocynaceae). Bp_5 190°.

Appel, H.H. *et al., Scientia (Valparaiso)*, 1961, **28**, 5-9; *CA*, **57**, 2332g

Sophora griffithii Alkaloid B A-425

Struct. unknown. Constit. of *Sophora griffithii.*

Primukhamedov, I. *et al., Rastit. Resur.*, 1969, **5**, 572-575; *CA*, **72**, 118549

Strychnos camptoneura Alkaloid B A-426

[58572-16-0]

Struct. unknown. Bisindole alkaloid. Alkaloid from *Strychnos camptoneura* (Loganiaceae). Mol. formula not reported (MW 622).

Verpoorte, R. *et al., Acta Pharm. Suec.*, 1975, **12**, 455-460 (*isol, uv, ir, ms*)

Thermopsis lanceolata Alkaloid B A-427

[78040-77-4]

Struct. unknown. Constit. of *Thermopsis lanceolata.*

▶AZ7675000

Chao, K.-S. *et al., CA*, 1981, **95**, 35461q (*isol, props*)

Alkaloid 241B A-428

[97380-36-4]

$C_{16}H_{35}N$ 241.459

Struct. unknown. Major alkaloid from skin extracts of the Madagascan frog *Mantella madagascariensis* (family Ranidae, subfamily Mantellinae). m/e 241 (15), 135 (45), 58 (100). Cannot be hydrogenated. No exchangeable hydrogen. Apparently lacks rings. Has not been detected in dendrobatid frogs.

Daly, J.W. *et al., Toxicon*, 1984, **22**, 905-919 (*isol, ms*)

C-Alkaloid BL A-429

$C_{40}H_{50}N_4O_2^{2\oplus}$ 618.861

An oxidn. prod. of *C*-Alkaloid D, A-476. Struct. unknown. Alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae).

▶Toxic (0.02 x Toxiferine).

Dichloride:

Cryst. + $2H_2O$. Dec. without melting, turning yellow, red then black. Deep-blue col. with $Ce(SO_4)_2$, becoming blue-green on standing.

Dipicrate: Mp 172-178°.

Schmidt, I. *et al., Helv. Chim. Acta*, 1960, **43**, 1218 (*isol, ir, uv*)
Gorman, A.A. *et al., Alkaloids (London)*, 1971, **1**, 200-338

Buxus Alkaloid BX6 A-430

Struct. unknown. Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 207-212°.

Döpke, W. *et al., Pharmazie*, 1969, **24**, 649; *CA*, **72**, 43929p (*isol*)

Buxus Alkaloid BX10 A-431

Struct. unknown. Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 221-224°.

Döpke, W. *et al., Pharmazie*, 1969, **24**, 649; *CA*, **72**, 43929p (*isol*)

***Chamaecytisus* Alkaloid C_1** **A-432**

$C_{15}H_{24}N_2O_2$ 264.367

Struct. unknown. Prob. a hydroxylupanine. Alkaloid from *Chamaecytisus frivaldskyanus, Chamaecytisus albus* and *Chamaecytisus calcareus* (Fabaceae). Mp 207-209°. $[\alpha]_D^{25}$ +59.2 (c, 0.38 in EtOH).

Daily, A. *et al., Planta Med.*, 1977, **32**, 380-383

***Chamaecytisus* Alkaloid C_2** **A-433**

$C_{12}H_{20}N_2O$ 208.303

Struct. unknown. Alkaloid from *Chamaecytisus austriacus, Chamaecytisus ciliatus* and *Chamaecytisus polytrichus* (Fabaceae). Mp 168-170°. $[\alpha]_D^{25}$ +38 (c, 0.4 in EtOH).

Daily, A. *et al., Planta Med.*, 1977, **32**, 380-383,

***Rauwolfia obscura* Alkaloid C_2** **A-434**

$C_{30}H_{34}N_4O$ 466.625

Bisindole alkaloid. Struct. unknown. Alkaloid from the leaves of *Rauwolfia obscura* (Apocynaceae). Mp 142-144°.

Timmins, P. *et al., Planta Med.*, 1975, **27**, 105-111 (*isol, uv, ir, pmr, ms*)

***Buxus* Alkaloid C** **A-435**

$C_{24}H_{42}N_2O$ 374.609

Struct. unknown. Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 212-214°. $[\alpha]_D$ +60 ($CHCl_3$). Props. similar to Cyclobuxamine H in C-846.

Schlittler, E. *et al., Helv. Chim. Acta*, 1949, **32**, 2209-2226 (*isol*)

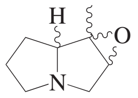
***C*-Alkaloid C** **A-436**

Struct. unknown. Alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). Characterised as picrate, dec. >270° without melting. Red-violet col. with $Ce(SO_4)_2$, becoming brown on standing.

Schmid, H. *et al., Helv. Chim. Acta*, 1952, **35**, 1864-1879; 1953, **36**, 102-121

***Crotalaria goreensis* Alkaloid C** **A-437**

Crotalaria goreensis *Base C*



Possible structure

$C_8H_{13}NO$ 139.197

Alkaloid from *Crotalaria goreensis* whole plant (Fabaceae). Bp_3 112-114°. $[\alpha]_D$ +9.3 (EtOH). pK_a 8.8. Conts. one C-Me group. Gives a dihydro deriv.

Culvenor, C.C.J. *et al., Aust. J. Chem.*, 1961, **14**, 284

***Dendrobates* Alkaloid 223C** **A-438**

[67217-78-1]

As *Dendrobates* Alkaloid 167A, A-354 with $R = C_5H_{11}$, $R' = CH_3$

$C_{15}H_{29}N$ 223.401

Tentative struct. Minor or trace alkaloid in skin extracts of *Dendrobates auratus, Dendrobates histrionicus* (various populations), *Dendrobates truncatus* and *Dendrobates* sp. of Colombia (Dendrobatidae). m/e 223(1), 222(2), 152(100). Cannot be hydrogenated.

Hydroxy (?)(1): **Dendrobates *Alkaloid 239E***

$C_{15}H_{29}NO$ 239.4

Trace alkaloid from skin extracts of *Dendrobates histrionicus* (Dendrobatidae). Mol. formula tentative. m/e 239(2), 238(3), 210(40), 152(100). Poss. a side-chain substd. deriv. of 223C. Cannot be hydrogenated.

Hydroxy (?)(2): **Dendrobates *Alkaloid 239F***

$C_{15}H_{29}NO$ 239.4

Trace alkaloid from skin extracts of *Dendrobates histrionicus* (Dendrobatidae). Mol. formula tentative. m/e 239(1), 168(100). Cannot be hydrogenated, forms *O*-Ac deriv.Poss. ring-substd. deriv. of 223C.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

***Dendrobates* Alkaloid 225C** **A-439**

$C_{15}H_{31}N$ 225.417

Struct. unknown. Tentatively proposed to be a 2-*n*-butyl-5-*n*-heptylpyrrolidine. Trace constit. in *Dendrobates histrionicus* (Dendrobatidae).

Daly, J.W. *et al., J. Nat. Prod.*, 1986, **49**, 265-280

***Dendrobates* Alkaloid 237C** **A-440**

$C_{16}H_{31}N$ 237.428

Struct. unknown. Minor alkaloid from skin extracts of *Dendrobates histrionicus* (Dendrobatidae). Mol. formula tentative; m/e 237 (2), 236 (1), 180 (100). Probably higher homologue of 223B. Cannot be hydrogenated.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

***Dendrobates* Alkaloid 239C** **A-441**

$C_{15}H_{29}NO$ 239.4

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates occultator* (Dendrobatidae). Mol. formula tentative; m/e 239 (2), 238 (3), 196 (100). Cannot be hydrogenated.

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

***Dendrobates* Alkaloid 251C** **A-442**

$C_{16}H_{29}NO$ 251.411

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates minutus* (Dendrobatidae). Mol. formula tentative; m/e 251 (2), 234 (4), 154 (100). H_2-deriv, m/e 253, 154.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

***Dendrobates* Alkaloid 283C** **A-443**

$C_{17}H_{33}NO_2$ 283.453

Struct. unknown. A major alkaloid from skin extracts of *Dendrobates histrionicus* and *Dendrobates occultator* (Dendrobatidae). m/e 283 (<1), 282 (1), 240 (5), 226 ($C_{13}H_{24}NO_2$, 28), 224 ($C_{15}H_{30}N$, 10), 166 ($C_{11}H_{20}N$, 60), 126 ($C_8H_{16}N$, 100). Cannot be hydrogenated.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

***Dendrobates* Alkaloid 307C** **A-444**

$C_{19}H_{33}NO_2$ 307.475

Struct. unknown. Minor alkaloid from skin extracts of *Dendrobates lehmanni* and *Dendrobates pumilio* (Dendrobatidae). m/e 307 (9), 290 (11), 182 (62), 70 (100). H_4-deriv, m/e 311 (3), 294 (3), 268 (5), 236(2), 110 (30), 84 (100), 70 (35).

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

***Dendrobates* Alkaloid 309C** **A-445**

$C_{19}H_{35}NO_2$ 309.491

Struct. unknown. Minor alkaloid from skin extracts of an undescribed *Dendrobates* sp. from Panama (Dendrobatidae). Mol. formula tentative; m/e 309 (3), 308 (2), 292 (1), 280 (4), 266 (4), 194 (15), 166 (100), 70(90). H_2-deriv, m/e 311 (3), 110 (25), 84(100), 70 (30).

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

***Erythrophleum* Alkaloid C** **A-446**

Struct. unknown. Alkaloid from the bark of *Erythrophleum couminga* (Fabaceae). Cryst. (petrol). Mp 116°. Readily dec. Possibly an artifact.

Cronlund, A. *et al., Acta Pharm. Suec.*, 1975, **12**, 467-478 (*isol, uv, ir, pmr, ms*)

***Gentiana macrophylla* Alkaloid C** **A-447**

Struct. unknown. Mol. formula not recorded. Monoterpene alkaloid. Alkaloid from the roots of *Gentiana macrophylla* (Gentianaceae). Cryst. (Me_2CO). Mp 206-208°.

Fu, F.-Y. *et al., Yaoxue Xuebao*, 1958, **6**, 198-203; *CA*, **53**, 8310b (*isol, uv*)

***Leucojum* Alkaloid C** **A-448**

Leucojum *Base C*

$C_{16}H_{17}NO_5$ 303.314

Amaryllidaceae alkaloid. Struct. unknown. Isol. from *Leucojum* sp.

(Amaryllidaceae). Mp 185-186°. $[\alpha]_D$ -29 ($CHCl_3$).

Raffauf, R.F. *et al., Handb. Alkaloids Alkaloid-Containing Plants*, Wiley, 1970, 284

Mantella Alkaloid 205C A-449

Struct. and MF unknown. Trace alkaloid from skin extracts of one population of the Madagascan frog *Mantella madagascariensis.*

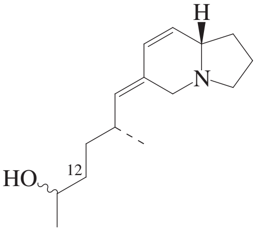
Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016 (*isol, ms*)

Mantella Alkaloid 211C A-450

Struct. and MF unknown. Trace alkaloid from skin extracts of the Madagascan frog *Mantella laevigata*.

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

Mantella Alkaloid 235C A-451



$C_{15}H_{25}NO$ 235.369

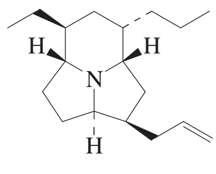
Structure revised in 2005. Alkaloid from skin extracts of the Madagascan frogs *Mantella aurantiaca*, *Mantella madagascariensis* and *Mantella crocea*.

Ketone: **Mantella** ***Alkaloid 233F***
$C_{15}H_{23}NO$ 233.353
Trace alkaloid from skin extracts of *Mantella madagascariensis, Mantella aurantiaca* and *Mantella crocea*.

12ξ-Hydroxy: **Mantella** ***Alkaloid 251G***
$C_{15}H_{25}NO_2$ 251.368
Alkaloid from a *Mantella* sp. Tentative struct. assigned.

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)
Andriamaharavo, N.R. *et al., J. Nat. Prod.*, 2005, **68**, 1743-1748 (*synth, ir, pmr, ms*)

Mantella Alkaloid 261C A-452



$C_{18}H_{31}N$ 261.45
Major alkaloid from skin extracts of the frog *Mantella betsileo*.

Dihydro(?): **Mantella** ***Alkaloid 263G***
$C_{18}H_{33}N$ 263.465
Alkaloid from skin extracts of *Mantella betsileo*.

Didehydro(?): Mantella *Alkaloid 259D*
$C_{18}H_{29}N$ 259.434
Alkaloid from the skin extracts of *Mantella betsileo.*

Hydroxy(?): **Mantella** ***Alkaloid 277G***
$C_{18}H_{31}NO$ 277.449
Alkaloid from the skin extracts of *Mantella betsileo*.

Hydroxy(?): **Mantella** ***Alkaloid 277H***
$C_{18}H_{31}NO$ 277.449
Alkaloid from the skin extracts of *Mantella betsileo*.

Kaneko, T. *et al., Heterocycles*, 2003, **59**, 745-757 (*isol, pmr, cmr, ms*)
Toyooka, N. *et al., Synlett*, 2005, 3109-3110 (*synth*)

Mantella Alkaloid 321C A-453

Allopumiliotoxin 321C

Struct. and MF unknown. Trace alkaloid from skin extracts of the Madagascan frog *Mantella betsileo*.

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ms*)

Salicornia herbacea Alkaloid C A-454

Struct. unknown. Alkaloid from *Salicornia herbacea* (Chenopodiaceae). Mp 236-238°.

Perchlorate: Mp 210-212°.

Picrate: Mp 117°.

Borkowski, B. *et al., Pharmazie*, 1965, **20**, 390-393; *CA*, **63**, 15223c

Stephania glabra Alkaloid C A-455

$C_{21}H_{25}NO_4$ 355.433

Struct. unknown. Not reported in further investigations of this species. Isol. from tubers of *Stephania glabra*. Cryst. (Me_2CO). Mp 182-183°. $[\alpha]_D$ +259 (c, 1 in EtOH). Conts. 3 OMe and 1 NMe group. λ_{max} 267 ; 304 (no solvent reported).

Hydrochloride: Mp 230-232°.

Kin, F.K. *et al., Khim. Prir. Soedin.*, 1965, **1**, 392-394; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 308-309
Cava, M.P. *et al., J.O.C.*, 1968, **33**, 2785-2789 (*Stephania glabra constits*)

Voacanga thouarsii Alkaloid C A-456

[50924-00-0]

$C_{42}H_{54}N_4O_{10}$ 774.909

Bisindole alkaloid. Struct. unknown. Alkaloid from the leaves of *Voacanga thouarsii* (Apocynaceae). Cryst. (MeOH). Mp 290-295° dec. $[\alpha]_D$ -282. Intense blue col. with HNO_3. λ_{max} 223 (log ε 4.57); 263 (log ε 4.1); 299 (log ε 4.17); 328 (log ε 4.21) (EtOH).

Rolland, Y. *et al., Phytochemistry*, 1973, **12**, 2039-2042 (*isol, uv, ir, pmr*)

Alkaloid C2 A-457

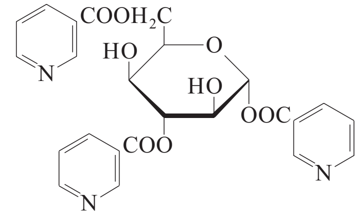
$C_{30}H_{34}N_4O$ 466.625

Prob. of Usambarine type. Struct. unknown. Alkaloid from the leaves of *Rauwolfia obscura* (Apocynaceae). Cryst. Mp 142-144°.

Timmins, P. *et al., Planta Med.*, 1975, **27**, 105-111 (*isol, uv, ir, pmr, ms*)

Alkaloid CB2 A-458

α-D-Glucopyranose 1,3,6-tri-3-pyridinecarboxylate, 9CI. 1,3,6-Tri-O-*nicotinoyl-α-D-glucopyranose*
[76129-64-1]

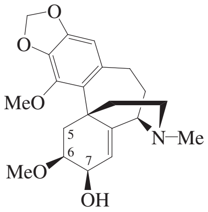


$C_{24}H_{21}N_3O_9$ 495.445
Alkaloid from stems of *Cryptolepis buchanani* (Asclepiadaceae). Mp 131-133°.

Dutta, S.K. *et al., Phytochemistry*, 1980, **19**, 1278 (*isol, uv, ir, pmr, ms, struct*)

Alkaloid CC 2 A-459

[35320-76-4]



Absolute Configuration

$C_{21}H_{27}NO_5$ 373.448
Alkaloid from the corms of *Colchicum cornigerum* (Liliaceae). Cryst. (EtOAc/Et_2O). Mp 172-174° (168-170°). $[\alpha]_D^{22}$ +40 (c, 0.48 in $CHCl_3$).

Ac: Mp 135-137°.

5,6-Didehydro, 7-ketone: ***Alkaloid CC 20***
[35320-75-3]
$C_{21}H_{23}NO_5$ 369.416
Alkaloid from the corms of *Colchicum cornigerum* (Liliaceae). Cryst. (EtOAc/Et_2O). Mp 210-212°. $[\alpha]_D^{22}$ +324 (c, 0.26 in $CHCl_3$).

Saleh, M. *et al., Coll. Czech. Chem. Comm.*, 1963, **28**, 3413 (*isol*)
Potěšilová, H. *et al., Coll. Czech. Chem. Comm.*, 1969, **34**, 3540 (*isol, uv, ir*)
Battersby, A.R. *et al., J.C.S.(C)*, 1971, 3514 (*uv, ir, pmr, cryst struct*)

Alkaloid CC 3 A-460

$C_{20}H_{25}NO_5$ 359.421

Struct. unknown. Alkaloid from the corms of *Colchicum cornigerum* (Liliaceae). Fine needles (EtOAc/Et_2O). Mp 197-199°. $[\alpha]_D^{22}$ +155 (c, 0.76 in $CHCl_3$).

El-Hamidi, A. *et al., Coll. Czech. Chem. Comm.*, 1962, **27**, 2111-2118 (*isol, uv, ir*)

Alkaloid CC 11 A-461

Mol. formula not reported. Struct. unknown. Alkaloid from the corms of *Colchicum cornigerum* (Liliaceae). Mp 251-253°.

Saleh, M. *et al., Coll. Czech. Chem. Comm.*, 1963, **28**, 3413-3423 (*isol*)

Alkaloid CC 13
A-462

Mol. formula not reported. Struct. unknown. Alkaloid from the seeds of *Colchicum cornigerum* (Liliaceae). Cryst. (MeOH). Mp 115-117°.

Saleh, M. *et al., Coll. Czech. Chem. Comm.*, 1963, **28**, 3413-3423 (*isol*)

Alkaloid CC 14
A-463

Struct. unknown. Mol. formula not reported. Alkaloid from the stems of *Colchicum cornigerum* (Liliaceae). Mp 182-185°.

Saleh, M. *et al., Coll. Czech. Chem. Comm.*, 1963, **28**, 3413-3423 (*isol*)

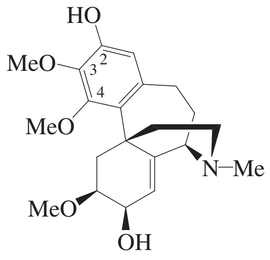
Alkaloid CC 23
A-464

Struct. unknown. MF = $C_{21-22}H_{23-27}NO_{5-6}$. Alkaloid from the corms of *Colchicum cornigerum* (Liliaceae). Mp 240-243°. $[\alpha]_D^{22}$ -22 (c, 0.2 in $CHCl_3$). $[\alpha]_D$ -4 (c, 0.3 in MeOH).

Potěšilová, H. *et al., Coll. Czech. Chem. Comm.*, 1969, **34**, 3540-3552 (*isol, uv, ir*)

Alkaloid CC 3b
A-465

[35320-77-5]



$C_{21}H_{29}NO_5$ 375.464

Probable struct. May be the O^4-de-Me, O^2-Me isomer. Alkaloid from the corms of *Colchicum cornigerum* (Liliaceae). Cryst. (EtOAc). Mp 210-212°. $[\alpha]_D^{22}$ +25 (c, 0.76 in $CHCl_3$).

Di-Ac: Mp 205-206°.

Potěšilová, H. *et al., Coll. Czech. Chem. Comm.*, 1969, **34**, 3540 (*isol, uv, ir*)

Battersby, A.R. *et al., J.C.S.(C)*, 1971, 3514 (*uv, ir, pmr, struct*)

Papaver Alkaloid $C_{21}H_{21}NO_6$
A-466

$C_{21}H_{21}NO_6$ 383.4

Struct. unknown. Alkaloid from the flowers of *Papaver rhoeas.* Yellow prisms. Mp 172-174°.

Awe, W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1957, **290**, 367-376 (*isol*)

Hortia Alkaloid $C_{22}H_{19}N_3O_3$
A-467

$C_{22}H_{19}N_3O_3$ 373.41

Struct. unknown. Alkaloid from the bark of *Hortia arborea*. Cryst. (Et_2O). Mp 136-139° Mp 191-194° (as hydrochloride).

Antonaccio, L.D. *et al., Ann. Acad. Bras. Cinc.*, 1956, **28**, 183-188; *CA*, **51**, 7385d (*isol*)

Alkaloid CN1
A-468

[126161-02-2]

$C_{23}H_{25}NO_5$ 395.454

Struct. unknown. Minor alkaloid from the aerial parts of *Corydalis nobilis* (Papaveraceae). Long thin needles (MeOH). Mp 210-211°.

Slavík, J. *et al., Coll. Czech. Chem. Comm.*, 1989, **54**, 2009-2020 (*isol, ms*)

Alkaloid CN2
A-469

[126161-13-5]

Struct. unknown. Minor alkaloid from the aerial parts of *Corydalis nobilis* (Papaveraceae). Light yellow prismatic needles (MeOH). Mp 260-261°. Ir 1660 cm^{-1} (CO), OH band absent.

Slavík, J. *et al., Coll. Czech. Chem. Comm.*, 1989, **54**, 2009-2020 (*isol, uv, ir*)

Alkaloid CR1
A-470

$C_{22}H_{34}NO_2^{\oplus}$ 344.516

Struct. unknown. Alkaloid from whole plants of *Consolida regalis.* Mp 288° (as iodide). $[\alpha]_D^{24}$ +29 (c, 0.2 in MeOH) (iodide). Contains a CO group (1760 cm^{-1}) and an OH group (3320 cm^{-1}). Prob. a quaternary C_{20}-diterpenoid alkaloid.

Slavík, J. *et al., Coll. Czech. Chem. Comm.*, 1987, **52**, 804-811 (*isol, uv, pmr, ms*)

Alkaloid CRB 11
A-471

$C_{21}H_{26}N_2O_3$ 354.448

Struct. unknown. Trace alkaloid from root of *Rauwolfia cumminsii* (Apocynaceae). Off-white amorph. powder. Prob. an indolenine.

Iwu, M.M. *et al., Planta Med.*, 1978, **34**, 390-396 (*isol, uv, ir, ms*)

Alkaloid CSA 3
A-472

CSA 3

Struct. unknown. Mol. formula not reported. Co-occurs with Cryptolepine and Indolo[3,2-*b*]quinoline, I-109. Could possibly be identical with Isocryptolepine in I-110. Alkaloid from roots of *Cryptolepis sanguinolenta* (Asclepiadaceae). Mp 300°.

Dwuma-Badu, D. *et al., J. Pharm. Sci.*, 1978, **67**, 433-434 (*isol*)

Rauwolfia obscura Alkaloid D_1
A-473

$C_{30}H_{34}N_4O$ 466.625

Struct. unknown. Bisindole alkaloid. Alkaloid from the leaves of *Rauwolfia obscura* (Apocynaceae). Mp 190-192°.

Timmins, P. *et al., Planta Med.*, 1975, **27**, 105-111 (*isol, uv, ir, ms*)

Rauwolfia obscura Alkaloid D_2
A-474

$C_{31}H_{36}N_4O$ 480.652

Struct. unknown. Bisindole alkaloid. Alkaloid from the leaves of *Rauwolfia obscura* (Apocynaceae). Amorph. yellow powder.

Timmins, P. *et al., Planta Med.*, 1975, **27**, 105-111 (*isol, uv, ms*)

Buxus Alkaloid D
A-475

Struct. unknown

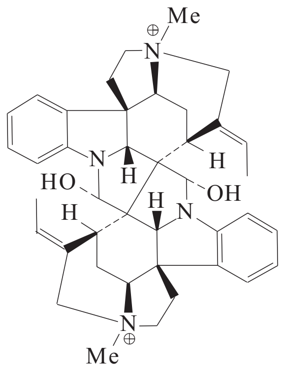
$C_{29}H_{50}N_2O$ 442.727

Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 182-183°. $[\alpha]_D$ +50 ($CHCl_3$).

Schlittler, E. *et al., Helv. Chim. Acta*, 1949, **32**, 2209-2226 (*isol*)

C-Alkaloid D
A-476

[6902-18-7]



$C_{40}H_{48}N_4O_2^{2\oplus}$ 616.845

Alkaloid from calabash curare (*Strychnos* spp.) and from *Strychnos castelneana* (Loganiaceae), also obt. by acid treatment of C-dihydrotoxiferine I. Shows low curarising activity. $[\alpha]_D$ -51 (50% Me_2CO aq.) (as dichloride). Characterised as dichloride and dipicrate, dec. >270° without melting. Red-violet col. with $Ce(SO_4)_2$ turning yellowish on standing.

▸ EY5200000

*Di-*N*-de-Me:* ***Bisnor*-C-*alkaloid D***

[62510-51-4]

$C_{38}H_{42}N_4O_2$ 586.775

Alkaloid from stem bark of *Strychnos dolichothyrsa* and from *Strychnos matopensis.* Poss. artifact. Tentative identification.

Schmid, H. *et al., Helv. Chim. Acta*, 1952, **35**, 1864; 1953, **36**, 102; 1954, **37**, 1993; 1961, **44**, 34 (*isol, uv, props*)

Battersby, A.R. *et al., Proc. Chem. Soc., London*, 1961, 413 (*struct*)

Delle Monache, F. *et al., J. Nat. Prod.*, 1970, **33**, 279 (*isol*)

Verpoorte, R. *et al., J. Nat. Prod.*, 1976, **39**, 357-362 (*Bisnor-*C*-alkaloid D*)

Massiot, G. *et al., Phytochemistry*, 1988, **27**, 3293-3304 (*isol, cmr*)

Cassia Alkaloid D
A-477

16-(5-Hydroxy-6-methyl-2-piperidinyl)-2,13-hexadecanediol, 9CI. 6-(4,15-Dihydroxyhexadecyl)-3-hydroxy-2-methylpiperidine

[38839-06-4]

$C_{22}H_{45}NO_3$ 371.602
Minor alkaloid from *Cassia carnaval* whole plant (Fabaceae). Oil. Cryst. salts could not be obt.

Lythgoe, D. *et al., An. Asoc. Quim. Argent.*, 1972, **60**, 317; *CA*, **77**, 164901 (*isol, uv, ir, ms*)

Coelidium **Alkaloid D** **A-478**

[11051-60-8]

$C_{16}H_{27}N_3$ 261.409

Struct. unknown. Alkaloid from *Coelidium fourcadei* dried leaves and branches (Fabaceae). Cryst. (hexane). Mp 138-139°. Interconverts with *Coelidium* Alkaloid E, A-497 in dil. acid. Cooccurs with Isotripiperideine, I-340 and α-Aldotripiperideine.

Arndt, R.R. *et al., J. S. Afr. Chem. Inst.*, 1968, **21**, 54-57 (*isol, ir, uv, pmr*)

Dendrobates **Alkaloid 223D** **A-479**

As *Dendrobates* Alkaloid 167A, A-354 with
$R = C_6H_{13}$, $R' = H$

$C_{15}H_{29}N$ 223.401

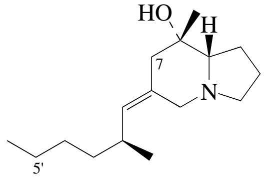
Tentative struct. Minor or trace alkaloid in skin extracts of *Dendrobates histrionicus* (various populations), *Dendrobates minutus, Dendrobates pumilio* and *Dendrobates truncatus* (Dendrobatidae). m/e 223(1), 222(2), 138(100). Cannot be hydrogenated.

Hydroxy (?): **Dendrobates *Alkaloid 239G***
$C_{15}H_{29}NO$ 239.4
Trace alkaloid from skin extracts of *Dendrobates histrionicus* (Dendrobatidae). Mol. formula tentative. m/e 239(1), 238(3), 138(100). Poss. side-chain hydroxy deriv. of 223D. Cannot be hydrogenated.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)
Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

Dendrobates **Alkaloid 251D** **A-480**

Octahydro-8-methyl-6-(2-methylhexylidene)-8-indolizinol, 9CI. Pumiliotoxin 251D
[73376-35-9]



$C_{16}H_{29}NO$ 251.411
A major alkaloid in skin extracts of the neotropical poison-frogs *Dendrobates tricolor, Dendrobates silverstonei, Dendrobates bombetes, Dendrobates* sp. (Colombia); minor or trace constit. of *Dendrobates auratus, Dendrobates histrionicus, Dendrobates lehmanni* and *Dendrobates minutus* (Dendrobatidae). $[\alpha]_D^{20}$ -8.5 (c, 1 in $CHCl_3$) (synthetic).

Hydrochloride:
Cryst. (hexane/EtOAc). Mp 206-206.5° (evac. capillary). $[\alpha]_D^{25}$ +32 (c, 0.5 in MeOH) (synthetic).

7β-Hydroxy: ***Allopumiliotoxin 267A***
[73376-38-2]
$C_{16}H_{29}NO_2$ 267.411
A major alkaloid in *Dendrobates auratus, Dendrobates azureus, Dendrobates fulguritus, Dendrobates granuliferus, Dendrobates lehmanni, Dendrobates leucomelas, Dendrobates minutus* (all populations), *Dendrobates tinctorius*; minor or trace constit. in *Dendrobates auratus* (different population), *Dendrobates histrionicus* and *Dendrobates pumilio* (Dendrobatidae). $[\alpha]_D^{25}$ +24.7 (c, 0.17 in MeOH).

5′ξ-Hydroxy: [94596-77-7]
$C_{16}H_{29}NO_2$ 267.411
Major alkaloid from skin of the Brazilian toad *Melanophyrniscus moreirae.* $[\alpha]_D^{25}$ +7.2 (c, 0.8 in MeOH). Has not been detected in dendrobatid frogs.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163 (*isol, ms*)
Daly, J.W. *et al., J.A.C.S.*, 1980, **102**, 830 (*isol, pmr, cmr, cryst struct, abs config*)
Overman, L.E. *et al., J.A.C.S.*, 1984, **106**, 4192 (*synth, pmr, cmr, ms*)
Tokuyama, T. *et al., Tetrahedron*, 1984, **40**, 1183 (*deriv*)
Daly, J.W. *et al., Toxicon*, 1984, **22**, 905 (*Pumiliotoxin 267C*)
Fox, D.N.A. *et al., J.A.C.S.*, 1991, **113**, 2652 (*synth*)
Honda, T. *et al., Heterocycles*, 1992, **34**, 1515 (*synth*)
Goldstein, S.W. *et al., J.O.C.*, 1992, **57**, 1179 (*Allopumiliotoxin 267A, synth*)
Aoyagi, S. *et al., J.A.C.S.*, 1993, **115**, 11393 (*Allopumiliotoxin 267A, synth*)
Honda, T. *et al., J.C.S. Perkin 1*, 1994, 2091 (*synth*)
Cossy, J. *et al., Synlett*, 1996, 909 (*synth*)
Martin, S.F. *et al., Tetrahedron*, 1999, **55**, 8905-8914 (*synth*)
Tang, X.-Q. *et al., J.A.C.S.*, 2000, **122**, 6950-6954 (*Allopumiliotoxin 267A, synth*)
Ni, Y. *et al., J.C.S. Perkin 1*, 2000, 3264-3266 (*synth*)
Comins, D.L. *et al., Org. Lett.*, 2001, **3**, 469-471 (*Allopumiliotoxin 267A, synth*)
Sudau, A. *et al., Eur. J. Org. Chem.*, 2002, 3315-3325 (*synth, pmr, cmr, ms*)
Woodin, K.S. *et al., J.O.C.*, 2007, **72**, 7451-7454 (*synth*)

Dendrobates **Alkaloid 253D** **A-481**

2-Allyl-5-(2,3-dihydroxypropyl)decahydroquinoline
As *Dendrobates* Alkaloid 219A, A-357 with
$R = –CH_2CH(OH)CH_2OH$
$C_{15}H_{27}NO_2$ 253.384
Alkaloid from skin extracts of the Colombian poison-frog *Dendrobates histrionicus* (Dendrobatidae).

Tokuyama, T. *et al., Tetrahedron*, 1986, **42**, 3453 (*isol, pmr, cmr, ms, struct*)
Spande, T.F. *et al., J. Nat. Prod.*, 1999, **62**, 5-21 (*pmr, cmr, occur*)

Dendrobates **Alkaloid 285D** **A-482**

Struct. unknown. Trace alkaloid from skin extracts of an undescribed *Dendrobates* sp. (Colombia)(Dendrobatidae). Mol. formula not known; m/e 285 (3), 270 (2), 256 (2), 180 (35), 140 (100). Atypical spectrum for a dendrobatid alkaloid.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates **Alkaloid 307D** **A-483**

$C_{18}H_{31}NO_3$ 309.448

Struct. unknown. Trace alkaloid from skin extracts of an undescribed *Dendrobates* sp. from Panama (Dendrobatidae). Mol. formula tentative; m/e 307 (8), 306 (5), 292 (3), 290 (5), 264 (4), 262 (11), 206 (11), 194(18), 166 (100), 70 (85). H_4-deriv, m/e 311, 110, 84, 70.

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Leucojum **Alkaloid D** **A-484**

Leucojum *Base D*
$C_{16}H_{19}NO_3$ 273.331

Amaryllidaceae alkaloid. Struct. unknown. Isol. from *Leucojum* sp. (Amaryllidaceae).

Raffauf, R.F. *et al., Handb. Alkaloids Alkaloid-Containing Plants*, Wiley, 1970, 284

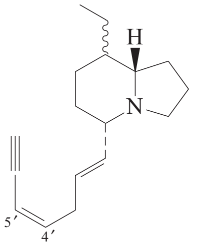
Mantella **Alkaloid 211D** **A-485**

Struct. and MF unknown. Trace alkaloid from skin extracts of the Madagascan frogs *Mantella* sp. cf. *madagascariensis, Mantella betsileo* and *Mantella laevigata*.

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

Mantella **Alkaloid 243D** **A-486**

8-Ethyl-5-(1,4-heptadien-6-ynyl)octahydroindolizine, 9CI. Indolizidine 243D
[151834-95-6]



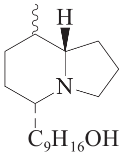
$C_{17}H_{25}N$ 243.391
Provisional struct. Minor or trace alkaloid from skin extracts of 2 populations of the Madagascan frog *Mantella madagascariensis.*

4′,5′-Dihydro: 8-Ethyl-5-(1-hepten-6-ynyl)octahydroindolizine, 9CI. **Mantella *Alkaloid 245C*.** *Indolizidine 245C*
[151805-29-7]
$C_{17}H_{27}N$ 245.407
Minor or trace alkaloid in 2 populations of *Mantella madagascariensis.* Provisional struct.

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016 (*isol, ir, ms*)

Mantella Alkaloid 279D A-487

(Octahydro-8-methyl-5-indolizinyl)-sec-nonenol, *9CI. Indolizidine 279D*
[151871-23-7]



$C_{18}H_{33}NO$ 279.465

Provisional struct. Secondary alcohol contg. a *Z*-double bond. Minor or trace alkaloid from skin extracts of 2 populations of the Madagascan frog *Mantella madagascariensis.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016 (*isol, ir, ms*)

Melodinus aeneus Alkaloid D A-488

Struct. unknown. Bisindole alkaloid. Alkaloid from *Melodinus aeneus* (Apocynaceae). No phys. props. recorded. M.W. = 534.

Baassou, S. *et al., Phytochemistry*, 1978, **17**, 1449-1450 (*isol*)

Narcissus Alkaloid D A-489

Narcissus *Base D*

$C_{17}H_{19}NO_3$ 285.342

Amaryllidaceae alkaloid. Approx. MF given (may be H_{21}). Struct. unknown. Isol. from *Narcissus* sp. (Amaryllidaceae). Prisms (Me_2CO). Mp 228-229° dec. $[\alpha]_D^{25}$ -175 (c, 0.2 in $CHCl_3$).

Boit, H.-G. *et al., Chem. Ber.*, 1957, **90**, 2197-2202 (*isol*)

Pandaca caducifolia Alkaloid D A-490

[$C_{40}H_{44\text{-}46}N_4O_{3\text{-}4}$]

Struct. unknown. Bisindole alkaloid. Alkaloid from *Pandaca caducifolia* (Apocynaceae). Noncryst. $[\alpha]_D$ +236 (MeOH). Alternative mol. formula $C_{40}H_{46}N_4O_4$.

Zeches, M. *et al., Phytochemistry*, 1975, **14**, 1122-1124 (*isol, uv, ir, pmr, ms*)

Salicornia herbacea Alkaloid D A-491

Struct. unknown. Alkaloid from *Salicornia herbacea* (Chenopodicaeae). Mp 178-180°.

Borkowski, B. *et al., Pharmazie*, 1965, **20**, 390-393; *CA*, **63**, 15223c

Stephania glabra Alkaloid D A-492

$C_{20}H_{25}NO_4$ 343.422

Struct. unknown. Isol. from tubers of *Stephania glabra*. Cryst. (C_6H_6). Mp 153-154°. Conts. 2 OMe and 1 NMe groups. Not reported in further investigations of this species. λ_{max} 265 (no solvent reported).

Hydrochloride: Mp 227-228°.

Hydrobromide: Mp 229-230°.

Kin, F.K. *et al., Khim. Prir. Soedin.*, 1965, **1**, 392-394; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 308-309 (*isol*)
Cava, M.P. *et al., J.O.C.*, 1968, **33**, 2785-2789 (*Stephania glabra constits*)

Alkaloid D1† A-493

Prob. of Usambarine type. Struct. unknown. Alkaloid from the leaves of *Rauwolfia obscura* (Apocynaceae). Off-white cryst. Mp 190-192°.

Timmins, P. *et al., Planta Med.*, 1975, **27**, 105-111 (*isol, uv, ir, pmr, ms*)

Alkaloid D2 A-494

Prob. of Usambarine type. Struct. unknown. Alkaloid from the leaves of *Rauwolfia obscura* (Apocynaceae). Amorph. yellow powder.

Timmins, P. *et al., Planta Med.*, 1975, **27**, 105-111

Alkaloid 267D A-495

[97380-35-3]

$C_{16}H_{29}NO_2$ 267.411

Struct. unknown. Alkaloid from skin extracts of the Australian frog *Pseudophryne semimarmorata* (Myobatrachidae) and the Madagascan frog *Mantella aurantiaca* (family Ranidae, subfamily Mantellinae). m/e 267 (13), 250 (10), 194 (16), 166 (100), 70(80). Forms H_2-deriv. Two exchangeable hydrogens. Has not been detected in dendrobatid frogs.

Daly, J.W. *et al., Toxicon*, 1984, **22**, 905-919 (*isol, ms*)

Buxus Alkaloid E A-496

$C_{27}H_{50}N_2O_3$ 450.704

Struct. unknown. Alkaloid from *Buxus balearica* (Buxaceae). Mp 287-289°. $[\alpha]_D^{20}$ +12 (c, 0.6 in $CHCl_3$/MeOH).

Kurakina, I.O. *et al., Khim. Prir. Soedin.*, 1969, **5**, 26-28; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 20-21 (*isol*)

Coelidium Alkaloid E A-497

[11051-61-9]

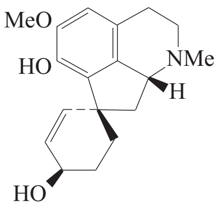
$C_{16}H_{27}N_3$ 261.409

Struct. unknown. Alkaloid from *Coelidium fourcadei* dried leaves and branches (Fabaceae). Cryst. (hexane). Mp 148-149°. Interconverts with *Coelidium* Alkaloid D, A-478 in dil. acid. Cooccurs with α-aldotripiperideine and Isotripiperideine, I-340.

Arndt, R.R. *et al., J. S. Afr. Chem. Inst.*, 1968, **21**, 54-57 (*isol, ir, uv, pmr*)

Croton linearis Alkaloid E A-498

[58206-97-6]



$C_{18}H_{23}NO_3$ 301.385

Belongs to diastereomeric series to alkaloids covered by Amuroline, A-957 and Cryprochine, C-781. Alkaloid from *Croton linearis* (Euphorbiaceae).

Di-Ac: Mp 190-193°. $[\alpha]_D^{26}$ -18 (c, 0.5 in MeOH).

4-Ketone, N*-de-Me:* ***Jacularine***
[20361-70-0]
$C_{17}H_{19}NO_3$ 285.342
Alkaloid from *Croton linearis* (Euphorbiaceae). Enantiomer of Isocrotsparinine in A-957.

Haynes, L.J. *et al., J.C.S.(C)*, 1966, 1680-1685 (*Alkaloid E*)
Stuart, K.L. *et al., Tet. Lett.*, 1968, 4473-4474 (*Jacularine*)
Casagrande, C. *et al., J.C.S. Perkin 1*, 1975, 1659-1663 (*stereochem*)

Dendrobates Alkaloid 223E A-499

$C_{14}H_{25}NO$ 223.358

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates lehmanni, Dendrobates occultator* and *Dendrobates tinctorius* (Dendrobatidae). Mol. formula tentative; m/e 223 (2), 222 (3), 168 (100). Possibly an analogue of *Dendrobates* Alkaloid 225, A-291 with double bond in side chain. H_2-deriv, m/e 223, 168.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 237E A-500

$C_{15}H_{27}NO$ 237.384

Struct. unknown. Trace alkaloid from skin extracts of *Dendrobates histrionicus* (Dendrobatidae). Mol. formula tentative; m/e 237 (1), 236 (3), 208 (70), 152 (100). Possibly a hydroxypumiliotoxin C. H_2-deriv, m/e 239, 152.

Daly, J.W. *et al., Toxicon*, 1978, **16**, 163-180 (*isol, ms, rev*)
Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Lycopodium Alkaloid E A-501

Lycopodium *Base E*

$C_{17}H_{25}NO_2$ 275.39

Struct. unknown. Alkaloid from *Lycopodium fawcettii* (Lycopodiaceae). Mp 267-269° dec. (as perchlorate).

Burnell, R.H. *et al., J.C.S.*, 1959, 3091 (*isol, ir*)

Muntafara sessilifolia Alkaloid E A-502

Struct. unknown. Bisindole alkaloid. Alkaloid from *Muntafara sessilifolia* (preferred genus name *Tabernaemontana*) (Apocynaceae). Other dimeric alkaloids isol. from *M. sessilifolia* designated F, I, J, N, O, P, Q and R. No phys. props. recorded.

Panas, J.M. *et al., Phytochemistry*, 1975, **14**, 1120-1122 (*isol*)

Pandaca caducifolia Alkaloid E A-503

$C_{40}H_{46}N_4O_4$ 646.828

Struct. unknown. Bisindole alkaloid. Alkaloid from *Pandaca caducifolia* (Apocynaceae). Noncryst. $[\alpha]_D$ -51 (MeOH).

Zeches, M. *et al., Phytochemistry*, 1975, **14**, 1122-1124 (*isol, uv, ir, pmr*)

Skytanthus acutus Alkaloid E A-504

$C_{10}H_{19}N$ 153.267

Struct. unknown. Monoterpene alkaloid. Alkaloid from *Skytanthus acutus* (Apocynaceae). Bp$_{1.5}$ 120-140°.

Appel, H.H. *et al., Scientia (Valparaiso)*, 1961, **28**, 5-9; *CA*, **57**, 2332g

Sophora microphylla Alkaloid E A-505

Sophora *Base E*

Struct. unknown. Alkaloid from *Sophora microphylla* (Fabaceae). Mp 168-171°.

Briggs, L.H. *et al., J.C.S.*, 1937, 1795 (*isol*)

Voacanga thouarsii Alkaloid E A-506

[50924-06-6]

$C_{43}H_{50}N_4O_7$ 734.891

Bisindole alkaloid. Struct. unknown. Alkaloid from the leaves of *Voacanga thouarsii* (Apocynaceae). Cryst. (MeOH). Mp 235-238°. $[\alpha]_D$ -140. Intense blue col. with HNO_3. λ_{max} 225 (log ϵ 4.66); 265 (log ϵ 4.08); 283 (sh) (log ϵ 3.96); 291 (sh) (log ϵ 3.9) (EtOH).

Rolland, Y. *et al., Phytochemistry*, 1973, **12**, 2039-2042 (*isol, uv, ir, pmr*)

Buxus Alkaloid F A-507

Struct. unknown. Alkaloid from *Buxus wallichiana* (Buxaceae). Mp 190°. $[\alpha]_D^{28}$ +26.6 (c, 0.76 in EtOH). MW 442.

Vassová, A. *et al., Pharmazie*, 1970, **25**, 363; *CA*, **73**, 127748n

Dendrobates Alkaloid 223F A-508

$C_{14}H_{25}NO$ 223.358

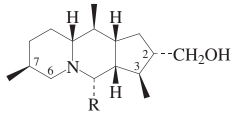
Struct. unknown. Trace alkaloid from skin extracts of an undescribed *Dendrobates* sp. from Panama (Dendrobatidae). Mol. formula tentative; m/e 223 (1), 138 (100). H_2-deriv, m/e 225, 182.

Daly, J.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1982, **41**, 205 (*ms, rev*)

Dendrobates Alkaloid 251F A-509

*Dodecahydro-3,7,10-trimethylcyclopenta[*b*]quinolizine-2-methanol, 9CI. Indolizidine 251F*

[142543-01-9]



Absolute Configuration

R = H

$C_{16}H_{29}NO$ 251.411

Major alkaloid from the skin extracts of the Colombian dendrobatid frog *Minyobates bombetes*. Pale yellow oil. $[\alpha]_D$ -11.1 (c, 0.96 in MeOH).

*Aldehyde: Dodecahydro-3,7,10-trimethylcyclopenta[*b*]quinolizine-2-carboxaldehyde, 9CI.* **Dendrobates *Alkaloid 249B*.** *Indolizidine 249B*
[142543-05-3]
$C_{16}H_{27}NO$ 249.395
Alkaloid from *Minyobates bombetes*. Tentative struct.

2,3,6,7-Tetradehydro: **Dendrobates *Alkaloid 247***
[142543-06-4]
$C_{16}H_{25}NO$ 247.38
Alkaloid from *Minyobates bombetes*. Tentative struct.

2,3,6,7-Tetradehydro, aldehyde: **Dendrobates *Alkaloid 245***
[142543-07-5]
$C_{16}H_{23}NO$ 245.364
Alkaloid from *Minyobates bombetes*. Tentative struct.

*Deoxy: Dodecahydro-2,3,7,10-tetramethylcyclopenta[*b*]quinolizine, 9CI.* Dendrobates *Alkaloid 235H. Indolizidine 235H*
[142543-02-0]
$C_{16}H_{29}N$ 235.412
Alkaloid from *Minyobates bombetes*. Tentative struct.

*Deoxy, 2ξ-hydroxy: Dodecahydro-2,3,7,10-tetramethylcyclopenta[*b*]quinolizin-2-ol, 9CI.* **Dendrobates *Alkaloid 251J*.** *Indolizidine 251J*
[142543-08-6]
$C_{16}H_{29}NO$ 251.411
Alkaloid from *Minyobates bombetes*. Tentative struct.

2-Epimer: **Dendrobates *Alkaloid 251F′*.** *Indolizidine 251F′*
[142631-46-7]
$C_{16}H_{29}NO$ 251.411
Alkaloid from *Minyobates bombetes*. Tentative struct.

*Homologue ($R = CH_3$): Dodecahydro-3,4,7,10-tetramethylcyclopenta[*b*]quinolizine-2-methanol, 9CI.* **Dendrobates *Alkaloid 265B*.** *Indolizidine 265B*
[142543-03-1]
$C_{17}H_{31}NO$ 265.438
Alkaloid from *Minyobates bombetes*. Tentative struct.

*Homologue ($R = CH_2CH_3$): 4-Ethyldodecahydro-3,7,10-trimethylcyclopenta[*b*]quinolizine-2-methanol, 9CI.* **Dendrobates *Alkaloid 279B*.** *Indolizidine 279B*
[142543-04-2]
$C_{18}H_{33}NO$ 279.465
Alkaloid from *Minyobates bombetes*. Tentative struct.

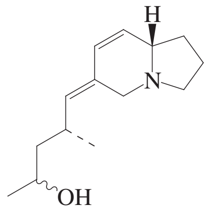
*Homologue ($R = CH_2CH_3$), deoxy, 2ξ-hydroxy: 4-Ethyldodecahydro-2,3,7,10-tetramethylcyclopenta[*b*]quinolizin-2-ol, 9CI.* **Dendrobates *Alkaloid 279C*.** *Indolizidine 279C*
[142543-09-7]
$C_{18}H_{33}NO$ 279.465
Alkaloid from *Minyobates bombetes*. Tentative struct.

Spande, T.F. *et al., J. Nat. Prod.*, 1992, **55**, 707-722 (*isol, pmr, ms*)

Taber, D.F. *et al., J.A.C.S.*, 1995, **117**, 5757-5762 (*synth, pmr, cmr*)

Wrobleski, A. *et al., J.A.C.S.*, 2004, **126**, 5475-5481 (*synth*)

Mantella Alkaloid 221F A-510



$C_{14}H_{23}NO$ 221.342

Structure tentatively reassigned in 2005. Trace alkaloid from skin extracts of the Madagascan frog *Mantella aurantiaca*.

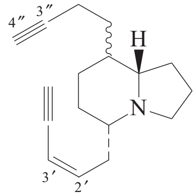
Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ms*)

Adriamaharavo, N.R. *et al., J. Nat. Prod.*, 2005, **68**, 1743-1748 (*struct*)

Mantella Alkaloid 241F A-511

8-(3-Butynyl)octahydro-5-(2-penten-4-ynyl)indolizine, 9CI. Indolizidine 241F

[151805-25-3]



$C_{17}H_{23}N$ 241.375

Provisional struct. Minor alkaloid from skin extracts of 2 populations of the Madagascan frog *Mantella madagascariensis.*

2′,3′-Dihydro: 8-(3-Butynyl)octahydro-5-(4-pentynyl)indolizine, 9CI. **Mantella *Alkaloid 243B*.** *Indolizidine 243B*
[151805-26-4]
$C_{17}H_{25}N$ 243.391
Trace alkaloid in one population of *Mantella madagascariensis*. Provisional struct.

3″,4″-Dihydro: 8-(3-Butenyl)octahydro-5-(2-penten-4-ynyl)indolizine, 9CI. **Mantella *Alkaloid 243C*.** *Indolizidine 243C*
[151805-27-5]
$C_{17}H_{25}N$ 243.391
Minor or trace alkaloid in 2 populations of *Mantella madagascariensis*. Provisional struct.

2′,3′,3″,4″-Tetrahydro: 8-(3-Butenyl)octahydro-5-(4-pentynyl)indolizine, 9CI. **Mantella *Alkaloid 245B*.** *Indolizidine 245B*
[151805-28-6]
$C_{17}H_{27}N$ 245.407

Trace alkaloid in 1 population of *Mantella madagascariensis*. Provisional struct.

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016 (*isol, ir, ms*)

Mantella Alkaloid 249F A-512

Homopumiliotoxin 249F

Struct. and MF unknown. Trace alkaloid from skin extracts of one population of the Madagascan frog *Mantella madagascariensis.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

Mantella Alkaloid 265F A-513

$C_{16}H_{27}NO_2$ 265.395

Struct. unknown. May be related to alkaloids of the 235C class. Trace alkaloid from skin extracts of the Madagascan frog *Mantella aurantiaca*.

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ms*)

Mantella Alkaloid 281F A-514

Struct. unknown. Probably belongs to the pumiliotoxin A class of alkaloid (see Pumiliotoxin A, P-791). Alkaloid from skin extracts of two populations of the Madagascan frog *Mantella madagascariensis.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

Pandaca caducifolia Alkaloid F A-515

$C_{40}H_{46}N_4O_4$ 646.828

Struct. unknown. Bisindole alkaloid. Alkaloid from *Pandaca caducifolia* (Apocynaceae). Noncryst. $[\alpha]_D$ +56 (MeOH).

Zeches, M. *et al., Phytochemistry*, 1975, **14**, 1122-1124 (*isol, uv, ir, pmr*)

Lycopodium Alkaloid G A-516

Lycopodium *Base G*

$C_{18}H_{27}NO_3$ 305.416

Struct. unknown. Alkaloid from *Lycopodium fawcettii* (Lycopodiaceae). Mp 198-200° (as perchlorate).

Burnell, R.H. *et al., J.C.S.*, 1959, 3091 (*isol, ir*)

Mantella Alkaloid 207G A-517

Homopumiliotoxin 207G

Struct. and MF unknown. Trace alkaloid from skin extracts of the Madagascan frog *Mantella viridis.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ms*)

Pandaca caducifolia Alkaloid G A-518

$C_{40}H_{46}N_2O_4$ 618.814

Struct. unknown. Bisindole alkaloid. Alkaloid from *Pandaca caducifolia* (Apocynaceae). Noncryst. $[\alpha]_D$ +35 (MeOH).

Zeches, M. *et al., Phytochemistry*, 1975, **14**, 1122-1124 (*isol, uv, ir, pmr*)

Voacanga thouarsii Alkaloid G A-519

[50923-99-4]

$C_{42}H_{50}N_4O_5$ 690.881

Bisindole alkaloid. Struct. unknown. Alkaloid from the leaves of *Voacanga thouarsii* (Apocynaceae). Cryst. (Et_2O). Mp 280-285° dec. $[\alpha]_D$ +46. Pink col. with HNO_3. λ_{max} 221 (log ϵ 4.63); 260 (log ϵ 4.29); 298 (log ϵ 3.7) (EtOH).

Rolland, Y. *et al., Phytochemistry*, 1973, **12**, 2039-2042 (*isol, uv, ir, pmr*)

Alkaloid 251G A-520

[97380-38-6]

$C_{15}H_{25}NO_2$ 251.368

Struct. unknown. Alkaloid from skin extracts of the Madagascan frog *Mantella aurantiaca* (family Ranidae, subfamily Mantellinae). m/e 251 (26), 250 (45), 162 (100). Forms H_2-deriv. Two exchangeable hydrogens. Hydroxy congener of Alkaloid 235C. Has not been detected in dendrobatid frogs.

Daly, J.W. *et al., Toxicon*, 1984, **22**, 905-919 (*isol, ms*)

Alkaloid GB14 A-521

$C_{24}H_{33}NO_5$ 415.528

Struct. unknown. Alkaloid from the bark of *Himantandra belgraveana* (*Galbulimima belgraveana*) (Himantandraceae). Prisms + $1H_2O$ (Me_2CO/heptane). Mp 106°.

Binns, S.V. *et al., Aust. J. Chem.*, 1965, **18**, 569-573 (*isol*)

Alkaloid GB15 A-522

$C_{22}H_{35}NO_3$ 361.523

Struct. unknown. Alkaloid from the bark of *Himantandra* (*Galbulimima*) *belgraveana* (Himantandraceae). Needles (C_6H_6). Mp 230°. $[\alpha]_D$ +58 (c, ca. 1 in $CHCl_3$).

Binns, S.V. *et al., Aust. J. Chem.*, 1965, **18**, 569-573 (*isol*)

Alkaloid GB16 A-523

$C_{20}H_{27}NO_2$ 313.439

Struct. unknown. Alkaloid from the bark of *Himantandra* (*Galbulimima*) *belgraveana* (Himantandraceae). Prisms (EtOAc). Mp 203°. $[\alpha]_D$ +550 (c, ca. 1 in $CHCl_3$).

Binns, S.V. *et al., Aust. J. Chem.*, 1965, **18**, 569-573 (*isol*)

Alkaloid GB17 A-524

$C_{21}H_{31}NO_3$ 345.481

Struct. unknown. Alkaloid from the bark of *Himantandra* (*Galbulimima*) *baccata* (Himantandraceae). Needles + $1H_2O$ (MeOH aq.). Mp 115°. $[\alpha]_D$ -21 (c, ca. 1 in $CHCl_3$).

Binns, S.V. *et al., Aust. J. Chem.*, 1965, **18**, 569-573 (*isol*)

Alkaloid GB18 A-525

$C_{22}H_{33}NO_3$ 359.508

Struct. unknown. Alkaloid from the bark of *Himantandra baccata* (preferred genus name *Galbulimima*) (Himantandraceae). Prisms (heptane). Mp 120°. $[\alpha]_D$ +37 (c, ca. 1 in $CHCl_3$).

Binns, S.V. *et al., Aust. J. Chem.*, 1965, **18**, 569-573 (*isol*)

Gentiana Alkaloid II A-526

Struct. unknown. Monoterpene alkaloid. Alkaloid from *Gentiana asclepiadea, Gentiana bulgarica, Gentiana cruciata, Gentiana lutea* and *Gentiana punctata* (Gentianaceae).

Mollov, N.M. *et al., Dokl. Bulg. Akad. Nauk*, 1965, **18**, 947; *CA*, **64**, 10084h (*isol, ir*)

Cordell, G.A. *et al., Alkaloids (Academic Press)*, 1977, **16**, 431 (*rev*)

Sternbergia Alkaloid III A-527

Sternbergia *Base III*

Amaryllidaceae alkaloid. Struct. unknown. Isol. from *Sternbergia fischeriana* (Amaryllidaceae). Mp 212-213°. Opt. inactive, mol. formula not recorded.

Hydrobromide: Mp 174-175°.

Picrate: Mp 217-219°.

Proskurnina, N.F. *et al., Chem. Zentralbl.*, 1954, **125**, 8353 (*isol*)

Solanum Alkaloid IV A-528

Struct. unknown. A glycoalkaloid cont. NH, OH and conjugated C=O. Isol. from epigeal parts of *Solanum nigrum* (Solanaceae). Cryst. (MeOH). Mp 320-325°. Cooccurs with Solasonine, Solamargine and β-Solamargine (see Spirosol-5-en-3-ol, S-456).

Aslanov, S.M. *et al., Khim. Prir. Soedin.*, 1971, **7**, 674; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 658

Ungernia Alkaloid IV A-529

Ungernia *Base IV*

Amaryllidaceae alkaloid. Struct. unknown. Isol. from the leaves of *Ungernia minor* (Amaryllidaceae). Cryst. (MeOH). Mp 193-194°.

Normatov, M. *et al., Uzb. Khim. Zh.*, 1965, **9**, 25-30; *CA*, **63**, 7061f (*isol*)

Gentiana cruciata Alkaloid IVb A-530

$C_{10}H_{16}N_2O_7$ 276.246

Struct. unknown. Monoterpene alkaloid. Alkaloid from *Gentiana cruciata* (Gentianaceae). Mp 138-140°.

Marekov, N. *et al., Dokl. Bulg. Akad. Nauk*, 1965, **18**, 999-1002; *CA*, **64**, 11270a (*isol, ir*)

Cordell, G.A. *et al., Alkaloids (Academic Press)*, 1977, **16**, 431-510 (*rev*)

Lycopodium annotinum Alkaloid IX A-531

Lycopodium *Base IX*

$C_{17}H_{25}NO_2$ 275.39

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae).

Methiodide: Mp 324°. $[\alpha]^{20}_{D}$ -49.8.

Methochloride: Mp 274°.

Methoperchlorate: Mp 316°.

Methopicrate: Mp 78-80°.

Achmatowicz, O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1958, **32**, 485 (*isol, uv*)

C-Alkaloid J A-532

$C_{19}H_{21}N_2$ 277.388

Struct. unknown. Alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). Mp 260° dec. (as picrate). Red-orange col. with $Ce(SO_4)_2$.

Kebrle, J. *et al., Helv. Chim. Acta*, 1953, **36**, 102-121 (*isol, uv*)

Mantella Alkaloid 207J A-533

Struct. and MF unknown. Possibly a homologue of Precoccinelline in D-886. Trace alkaloid from skin extracts of one population of the Madagascan frog *Mantella madagascariensis.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

Mantella Alkaloid 235J A-534

Homopumiliotoxin 235J

Struct. and MF unknown. Trace alkaloid from skin extracts of one population of the Madagascan frog *Mantella madagascariensis.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

Mantella Alkaloid 235K A-535

Struct. and MF unknown. Considered to be a tricyclic alkaloid. Trace alkaloid from skin extracts of the Madagascan frog *Mantella betsileo.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ms*)

Alkaloid K2 A-536

$C_{21}H_{27}NO_6$ 389.447

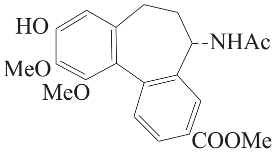
Struct. unknown. Alkaloid from the above-ground parts of *Colchicum kesselringii* (Liliaceae). Mp 226-228°.

Methiodide: Mp 247-249°.

Yusupov, M.K. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 1682 (*isol*)

Alkaloid K4 A-537

2-Demethylallocolchicine



$C_{21}H_{23}NO_6$ 385.416

(S)-form

Alkaloid from the above-ground parts of *Colchicum kesselringii* (Liliaceae). Mp 238-240° (natural) Mp 259-260° (semisynthetic). $[\alpha]^{20}_{D}$ -152 (c, 0.92 in MeOH) (semisynthetic).

Ac: Cryst. ($Et_2O/CHCl_3$). Mp 230-232°. $[\alpha]^{22}_{D}$ -150 (c, 1.0 in MeOH).

Me ether: ***Allocolchicine***. *Suhailamine. Alkaloid K3*

[641-28-1]

$C_{22}H_{25}NO_6$ 399.443

Alkaloid from the flowers of *Colchicum autumnale*, from *Colchicum decaisnei* and above ground parts of *Colchicum kesselringii* (Liliaceae). Cryst. ($Et_2O/CHCl_3$) or amorph. solid. Mp 257-258°. $[\alpha]^{22}_{D}$ -150 (c, 1.2 in MeOH) (semisynthetic). First descr. as Alkaloid K3 without abs. config. or opt. rotn. Suhailamine (1991) assigned (*S*)-config. However, spectroscopic and phys. props. of authentic Allocolchicine differ from those of Suhailamine and therefore the true struct. of the latter remains unclear.

▶ HO7884000

Yusupov, M.K. *et al., Zh. Obshch. Khim.*, 1964, **34**, 1677-1680; *J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 1686-1688 (*isol struct*)

Yusupov, M.K. *et al., Khim. Prir. Soedin.*, 1973, **9**, 194-196; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 188-189

Mackay, M.F. *et al., Acta Cryst. C*, 1989, **45**, 795-799 (*Allocolchicine, cryst struct*)

Abu Zarga, M.H. *et al., J. Nat. Prod.*, 1991, **54**, 936-940 (*Suhailamine*)

Banwell, M.G. *et al., Chem. Comm.*, 1994, 2647-2649 (*Suhailamine*)

Leblanc, M. *et al., Org. Lett.*, 2005, **7**, 2849-2852 (*synth*)

Alkaloid K5 A-538

$C_{19}H_{25}NO_4$ 331.411

Struct. unknown. Alkaloid from the above-ground parts of *Colchicum kesselringii* (Liliaceae). Mp 224-226°.

Hydrochloride: Mp 239-241°.

Methiodide: Mp 278-280°.

Yusupov, M.K. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 1682 (*isol*)

Alkaloid K6 A-539

Struct. unknown. Alkaloid from the above-ground parts of *Colchicum kesselringii* (Liliaceae).

Methiodide: Mp 253-254°.

Yusupov, M.K. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 1682 (*isol*)

Alkaloid K7 A-540

$C_{21}H_{29}NO_4$ 359.464

Struct. unknown. Alkaloid from the above-ground parts of *Colchicum kesselringii* (Liliaceae). Mp 144-146°.

Hydrochloride: Mp 232-234°.

Methiodide: Mp 247-248°.

Yusupov, M.K. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 1682 (*isol*)

Alkaloid K9 A-541

Struct. unknown. Alkaloid from the above-ground parts of *Colchicum kesselringii* (Liliaceae).

Methiodide: Mp 245-247°.

Yusupov, M.K. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 1682 (*isol*)

Alkaloid K10 A-542

$C_{18}H_{23}NO_4$ 317.384

Struct. unknown. Alkaloid from the above-ground parts of *Colchicum kesselringii* (Liliaceae). Cryst. (Me_2CO/MeOH). Mp 232-234°.

Hydrochloride: Mp 261-263°.

Methiodide: Mp 249-251°.

Yusupov, M.K. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 1682 (*isol*)

Alkaloid K11 A-543

Struct. unknown. Alkaloid from the above-ground parts of *Colchicum kesselringii* (Liliaceae). Mp 274-276°.

Yusupov, M.K. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 1682 (*isol*)

C-Alkaloid L A-544

Struct. unknown. Alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). Prisms (Me_2CO aq.) (as picrate). Mp 171° (picrate). Red col. with $Ce(SO_4)_2$.

Kebrle, J. *et al., Helv. Chim. Acta*, 1953, **36**, 102-121 (*isol, uv*)

Colubrina Alkaloid L A-545

$C_{37}H_{40}N_2O_6$ 608.733

Bisbenzylisoquinoline alkaloid. Struct. unknown. Alkaloid from the stem bark of *Colubrina faralaotra* ssp. *faralaotra* (Rhamnaceae).

Guinaudeau, H. *et al., Planta Med.*, 1975, **27**, 304-318 (*isol, uv, pmr, ms*)

Mantella Alkaloid 251L A-546

Homopumiliotoxin 251L

Struct. and MF unknown. Occurs mainly as the *O*-Ac deriv. Trace alkaloid from skin extracts of one population of the Madagascan frog *Mantella madagascariensis.*

Garraffo, H.M. *et al., J. Nat. Prod.*, 1993, **56**, 1016-1038 (*isol, ir, ms*)

Alkaloid L10 A-547

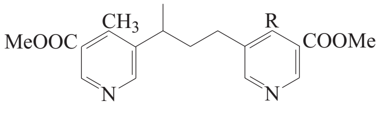
$C_{16}H_{27}NO$ 249.395

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae). Mp 223° (as perchlorate).

Manske, R.H.F. *et al., Can. J. Res., Sect. B*, 1943, **21**, 92-96 (*isol*)

Alkaloid LA 4 A-548

[116097-93-9]



R = H

$C_{19}H_{22}N_2O_4$ 342.394

Alkaloid artifact generated by NH_3 and secoiridoid glucoside from ripe fruits of the common privet *Ligustrum vulgare* (Oleaceae). Semi-solid. $[\alpha]^{20}_{D}$ -0.23 (c, 1.0 in EtOH).

Willems, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 229 (*isol, uv, ir, pmr, cmr, ms, struct*)

Alkaloid LA 5 A-549

[115531-75-4]

As Alkaloid LA 4, A-548 with

R = CH_3

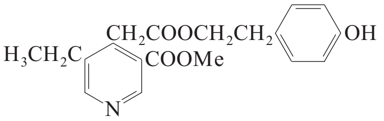
$C_{20}H_{24}N_2O_4$ 356.421

Alkaloid artifact generated by NH_3 and secoiridoid glucosides from ripe fruit of the common privet *Ligustrum vulgare* (Oleaceae). Semi-solid. $[\alpha]_D^{20}$ -0.39 (c, 1.0 in EtOH).

Willems, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 229 (*isol, uv, ir, pmr, cmr, ms, struct*)

Alkaloid LA 6 A-550

[113145-61-2]



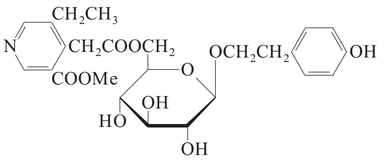
$C_{19}H_{21}NO_5$ 343.379

Alkaloid artifact generated by NH_3 and secoiridoid glucosides from ripe fruits of the common privet *Ligustrum vulgare* (Oleaceae). Needles (EtOAc/MeOH). Mp 115-116°.

Willems, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1987, **320**, 1245 (*isol, uv, ir, pmr, cmr, ms, struct*)

Alkaloid LA 9 A-551

[116057-84-2]



$C_{25}H_{31}NO_{10}$ 505.521

Alkaloid artifact generated by NH_3 and secoiridoid glucosides from ripe fruits of the common privet *Ligustrum vulgare* (Oleaceae). Cryst. (EtOAc/MeOH). Mp 64-66°. $[\alpha]_D^{20}$ -0.1 (c, 1.0 in EtOH).

Willems, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 357 (*isol, uv, ir, pmr, cmr, struct*)

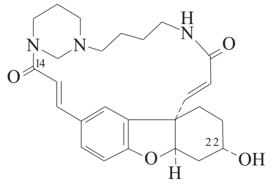
Alkaloid LB1 A-552

Prob. a spermidine related alkaloid. Struct. unknown. Minor alkaloid from the seeds of *Lunaria biennis* (Brassicaceae). Mp 220° dec.

Hairs, E. *et al., Bull. Acad. R. Med. Belg.*, 1909, 1042-1048; *CA*, 1892, **4**, 1042 (*isol*)

Alkaloid LBZ A-553

[38143-11-2]



$C_{26}H_{33}N_3O_4$ 451.564

CAS numbering shown. Minor alkaloid from the seeds of *Lunaria biennis* (Brassicaceae). Amorph.

22-Ketone: ***Alkaloid LBX***

[38143-10-1]

$C_{26}H_{31}N_3O_4$ 449.549

Minor alkaloid from the seeds of *Lunaria biennis* (Brassicaceae). Cryst. (MeOH/Me_2CO or MeOH/Et_2O). Mp 250° dec. $[\alpha]_D^{20}$ +201 (c, 0.6 in $CHCl_3$).

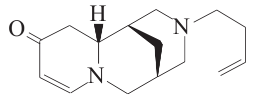
Doskotch, R.W. *et al., Experientia*, 1972, **28**, 382 (*struct*)

Poupat, C. *et al., Tetrahedron*, 1972, **28**, 3087 (*uv, ir, pmr, struct*)

Alkaloid LC2 A-554

*3-(3-Butenyl)-1,2,3,4,5,6,11,11*a*-octahydro-1,5-methano-10*H*-pyrido[1,2-*a*][1,5]diazocin-10-one, 9CI. 1,13-Didehydro-10,11-secomultiflorine. 11,12-Seco-12-dehydromultiflorine.* N*-Methylalbine (incorr.)*

[71635-26-2]



$C_{15}H_{22}N_2O$ 246.352

Struct. revised in 1988. Some isolates were prev. reported erroneously as *N*-methylalbine (see Albine, A-243). Alkaloid from the leaves and seeds of *Lupinus cosentinii*, *Lupinus albus* and *Lupinus formosus* (Fabaceae). Cryst. (cyclohexane). Mp 60°. $[\alpha]_D^{25}$ -520 (c, 1.0 in MeOH).

[97906-66-6 , 6822-63-5]

Beck, A.B. *et al., J. Nat. Prod.*, 1979, **42**, 385 (*isol, uv, ir, pmr, ms, struct*)

Wysocka, W. *et al., Planta Med.*, 1988, **54**, 522 (*cmr, ms, struct*)

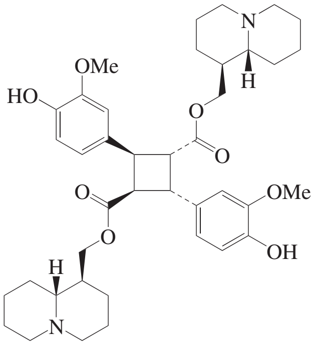
Brukwicki, T. *et al., J. Mol. Struct.*, 1989, **196**, 343 (*cmr, conform, bibl*)

Wyrzykiewicz, E. *et al., Org. Mass Spectrom.*, 1990, **25**, 453 (*ms*)

Dutkiewicz, G. *et al., Acta Cryst. C*, 1995, **51**, 1182 (*cryst struct*)

Alkaloid LC7 A-555

Alkaloid LV3†



Probable structure

$C_{40}H_{54}N_2O_8$ 690.875

Truxillate-type dimer of Epilupinyl trans-ferulate in E-95. Alkaloid from leaves of *Lupinus cosentinii* (Fabaceae). Cryst. (MeOH/$CHCl_3$). Mp 228°. $[\alpha]_D^{25}$ +23 (c, 1 in $CHCl_3$/MeOH 1:1).

Beck, A.B. *et al., J. Nat. Prod.*, 1979, **42**, 385 (*isol, struct, uv, ir, pmr, ms*)

Alkaloid LE1 A-556

$C_{28}H_{47}N_3O$ 441.699

Struct. unknown. Alkaloid from *Lycopodium erythraeum* (Lycopodiaceae).

MacLean, D.B. *et al., Alkaloids (Academic Press)*, 1985, **26**, 241

Alkaloid LO1 A-557

$C_{31}H_{39}N_3O_2$ 485.668

Struct. unknown. Alkaloid from *Lycopodium obtusifolium* (Lycopodiaceae).

MacLean, D.B. *et al., Alkaloids (Academic Press)*, 1985, **26**, 241

Alkaloid LO2 A-558

$C_{30}H_{49}N_3O$ 467.737

Struct. unknown. Alkaloid from *Lycopodium obtusifolium* (Lycopodiaceae).

MacLean, D.B. *et al., Alkaloids (Academic Press)*, 1985, **26**, 241

Alkaloid LO3 A-559

$C_{29}H_{49}N_3$ 439.726

Struct. unknown. Alkaloid from *Lycopodium obtusifolium* (Lycopodiaceae).

MacLean, D.B. *et al., Alkaloids (Academic Press)*, 1985, **26**, 241

Alkaloid LS14 A-560

$C_{30}H_{49}N_3O$ 467.737

Struct. unknown. Alkaloid from *Lycopodium saururus* (Lycopodiaceae).

MacLean, D.B. *et al., Alkaloids (Academic Press)*, 1985, **26**, 241

Alkaloid LV1† A-561

$C_{15}H_{22}N_2O$ 246.352

Not the same as Alkaloid LV1, A-562. Struct. unknown. Alkaloid from *Lupinus digitatus* (Fabaceae). Needles (Me_2CO/petrol). Mp 108-109°. $[\alpha]_D$ -314 (MeOH). Deep-red col. with $FeCl_3$.

Perchlorate:

Cream needles + ½H_2O (EtOH). Mp 160-162° dec. Cryst. with difficulty.

Methiodide:

Cream nodules (EtOH). Mp 246-248° dec.

Crow, W.D. *et al., Aust. J. Chem.*, 1955, **8**, 136-139; 1957, **10**, 177-181

Gladstones, J.S. *et al., J. R. Soc. West. Aust.*, 1958, **41**, 29

Alkaloid LV1† A-562

$C_{29}H_{45}N_3$ 435.695

Not the same as Alkaloid LV1, A-561. Struct. unknown. Alkaloid from *Lycopodium verticillatum* (Lycopodiaceae).

MacLean, D.B. *et al., Alkaloids (Academic Press)*, 1985, **26**, 241

Alkaloid LV2 A-563

$C_{15}H_{24}N_2O_2$ 264.367

Struct. unknown. Tentative mol. formula. Trace alkaloid from seeds of *Lupinus varius* (Fabaceae).

Crow, W.D. *et al., Aust. J. Chem.*, 1955, **8**, 136-139

Alkaloid LV3† A-564

$C_{20}H_{27}NO_4$ 345.438

Struct. unknown. Alkaloid from *Lupinus digitatus* (Fabaceae). Needles (MeOH). Mp 232-233° dec. Conts. one OMe group. λ_{max} 235 nm. Possibly the monomer of Alkaloid LC7, A-555.

Picrate:

Yellow needles (Me_2CO aq.). Mp 186°. Dec. sharply at 231°.

Crow, W.D. *et al., Aust. J. Chem.*, 1957, **10**, 177-181

Gladstones, J.S. *et al., J. R. Soc. West. Aust.*, 1958, **41**, 29

Alkaloid LV4 A-565

$C_{17}H_{23}NO_5$ 321.372

Provisional mol. formula. Struct. unknown. Alkaloid from *Lupinus digitatus* (Fabaceae). Needles ($CHCl_3$/petrol). Mp 235-237° dec.

Crow, W.D. *et al., Aust. J. Chem.*, 1957, **10**, 177-181

Gladstones, J.S. *et al., J. R. Soc. West. Aust.*, 1958, **41**, 29

Buxus Alkaloid M† A-566

See also *Buxus* Alkaloid M, A-567. Struct unknown. Alkaloid from *Buxus wallichiana* (Buxaceae). Mp 261°. $[\alpha]_D^{23}$ +27 (c, 0.33 in $CHCl_3$).

Vassová, A. *et al., Pharmazie*, 1970, **25**, 363-365; *CA*, **73**, 127748n

Buxus Alkaloid M† A-567

$C_{27}H_{46}N_2O$ 414.673

Struct. unknown. Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 203-205°. $[\alpha]_D$ -80 ($CHCl_3$).

Friedrich, W. *et al., Helv. Chim. Acta*, 1950, **33**, 873-878 (*isol*)

C-Alkaloid M A-568

$C_{20}H_{23}N_2O_2^{\oplus}$ 323.414

Struct. unknown. Minimum formula. Alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). Slowly developing yellow col. with $Ce(SO_4)_2$.

Asmis, H. *et al., Helv. Chim. Acta*, 1954, **37**, 1968-1973 (*isol, uv*)

Alkaloid MB 10 A-569

$C_{23}H_{30}N_2O_5$ 414.5

Struct. unknown. Alkaloid from roots of *Rauwolfia mombasiana* (Apocynaceae). Off-white amorph. powder. Conts. 2 OMe groups.

Iwu, M.M. *et al., Planta Med.*, 1980, **38**, 260-263 (*isol, uv, ir, ms*)

Buxus Alkaloid N A-570

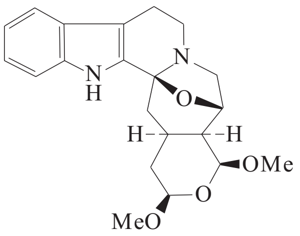
$C_{22}H_{35}NO_2$ 345.524

Struct. unknown. Poss. identical with Buxtauine M, B-482. Alkaloid from *Buxus sempervirens* (Buxaceae). Mp 178-179°. $[\alpha]_D$ +150 ($CHCl_3$). Props. corresp. to Buxtauine M, B-482.

Friedrich, W. *et al., Helv. Chim. Acta*, 1950, **33**, 873-878 (*isol*)

Alkaloid ND 370 A-571

[37304-95-3]



$C_{21}H_{26}N_2O_4$ 370.447

Alkaloid from the bark of *Nauclea diderrichii* (Rubiaceae). Cryst. by subl. Mp 209-211°.

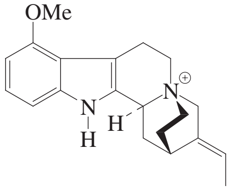
MacLean, S. *et al., Can. J. Chem.*, 1972, **50**, 1496; 1976, **54**, 1262 (*uv, ir, pmr, ms, struct*)

C-Alkaloid O A-572

19,20-Didehydro-9-methoxy-4,17-cyclocorynanium, 9CI

[86138-68-3]

[86138-69-4]



Absolute Configuration

$C_{20}H_{25}N_2O^{\oplus}$ 309.43

Quaternary alkaloid from calabash curare and *Strychnos guianensis* (Loganiaceae). Mp 288-289° dec. (as chloride). $[\alpha]_D^{22}$ -150 (c, 0.283 in 5%Py aq.) (as chloride). λ_{max} 227 (log ϵ 4.1); 266 (log ϵ 3.88); 282 (log ϵ 3.77); 291 (log ϵ 3.73) (MeOH).

Giesbrecht, E. *et al., Helv. Chim. Acta*, 1954, **37**, 1974-1982 (*isol*)

Borris, R.P. *et al., Helv. Chim. Acta*, 1983, **66**, 405 (*struct, spectra*)

Penelle, J. *et al., Phytochemistry*, 2000, **53**, 1057-1066; 2001, **58**, 619-626 (*isol, uv, ir, cd, pmr, cmr, activity*)

Alkaloid Or_2 A-573

Struct. unknown

Alkaloid from *Papaver orientale* and *Papaver pseudo-orientale* (Papaveraceae). Cryst. (petrol). Mp 124-127° (120-121°). Unstable, not obt. completely pure. m/e 333.

Délenk-Heydenreich, K. *et al., Pharmazie*, 1969, **24**, 635-645 (*isol, uv, ms*)

Shafiee, A. *et al., J. Pharm. Sci.*, 1975, **64**, 1570-1572 (*isol, uv, pmr*)

Baptisia Alkaloid P_2 A-574

$C_{11}H_{18}N_2O$ 194.276

Struct. unknown. Isol. from *Baptisia australis* and *Baptisia perfoliata*. Cryst. ($MeOH/Et_2O$). Mp 300°.

Perchlorate:

Needles (MeOH). Mp 198°.

Marion, L. *et al., J.A.C.S.*, 1948, **70**, 691-692; 3253-3254 (*isol*)

Oung-Boran, *et al., Planta Med.*, 1969, **17**, 301-318 (*isol*)

Baptisia Alkaloid P_4 A-575

Struct. unknown. Isol. from *Baptisia minor*. Oil. $Bp_{0.05}$ 175-200°.

Perchlorate:

Needles. Mp 286°.

Marion, L. *et al., J.A.C.S.*, 1948, **70**, 3472-3474 (*isol*)

C-Alkaloid P A-576

$C_{20}H_{23}N_2O^{\oplus}$ 307.414

Struct. unknown. Quaternary alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). Mp 224-232° (as picrate). Blue col. with $Ce(SO_4)_2$.

Giesbrecht, E. *et al., Helv. Chim. Acta*, 1954, **37**, 1974-1982 (*isol, uv*)

Lupinus Alkaloid P1 A-577

$C_{15}H_{22}N_2O$ 246.352

Tentative mol. form. Struct. unknown. Alkaloid from *Lupinus macounii* (Fabaceae). Small plates (EtOH/petrol). Mp 126° (sinters at 123°). Salts could not be obt. crystalline. Cooccurs with Anagyrine, A-970 and Lupanine, L-302.

Marion, L. *et al., J.A.C.S.*, 1946, **68**, 759-760

Lupinus Alkaloid P2 A-578

$C_{11}H_{18}N_2O$ 194.276

Tentative mol. formula. Lupine alkaloid. Struct. unknown. Alkaloid from *Baptisia australis* and *Baptisia perfoliata* (Fabaceae). Cryst. ($MeOH/Et_2O$). Mp 300°.

Perchlorate:

Needles (MeOH). Mp 198°.

Picrate(?): Mp 241° (sinters at 185°).

Marion, L. *et al., J.A.C.S.*, 1948, **70**, 691-692; 3253-3254 (*isol*)

Mucuna pruriens Alkaloid P A-579

Mucuna pruriens *Base P*

$C_{17}H_{26}NO_6$ 340.395

Struct. unknown. Alkaloid from *Mucuna pruriens* (Fabaceae). Bp 118-119°.

Picrate: Mp 100-101°.

Rakhit, S. *et al., Indian J. Pharm.*, 1956, **18**, 285; *CA*, **52**, 5748e (*isol*)

Alkaloid PAR 1 A-580

Struct. unknown. Mol. formula not recorded. Minor alkaloid from *Papaver argemone* (Papaveraceae). Prisms (MeOH). Mp 193-195°.

Táborská, E. *et al., Coll. Czech. Chem. Comm.*, 1988, **53**, 1845 (*isol, uv*)

Alkaloid PAR 2 A-581

Struct. unknown. Mol. formula not

recorded. Minor alkaloid from *Papaver argemone* (Papaveraceae). Prisms (MeOH). Mp 252-256°.

Táborská, E. *et al., Coll. Czech. Chem. Comm.*, 1988, **53**, 1845 (*isol, uv*)

Alkaloid PAR 3 **A-582**

Struct. unknown. Quaternary alkaloid. Mol. formula and counterion not specified. Minor alkaloid from *Papaver argemone* (Papaveraceae). Amorph.

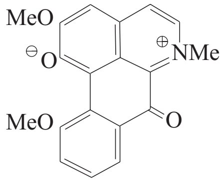
Táborská, E. *et al., Coll. Czech. Chem. Comm.*, 1988, **53**, 1845 (*isol, uv*)

Alkaloid PO3 **A-583**

*1-Hydroxy-2,11-dimethoxy-6-methyl-7*H*-dibenzo[*de,g*]quinolinium hydroxide inner salt, 9CI*

[27699-47-4]

[101064-66-8]



$C_{19}H_{15}NO_4$ 321.332

Alkaloid from *Papaver orientale* (Papaveraceae). Amorph.

Perchlorate: Mp 253-255°.

Preininger, V. *et al., CA*, 1967, **67**, 54290w (*isol*)

Preininger, V. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1969, **302**, 808 (*uv, ir, pmr*)

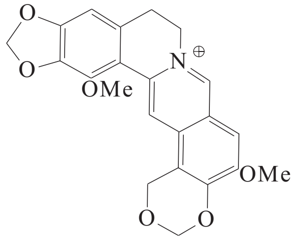
Saá, C. *et al., Tet. Lett.*, 1985, **26**, 4559 (*synth*)

Atanes, N. *et al., J.O.C.*, 1991, **56**, 2984 (*synth*)

Alkaloid PO4 **A-584**

Dehydroorientalidine

[23943-92-2]



$C_{22}H_{20}NO_6^{\oplus}$ 394.403

Alkaloid from *Papaver orientale, Papaver oreophilum, Papaver nudicaule* var. *leiocarpum, Papaver pyrenaicum* ssp. *rhoeaticum* and *Papaver alboroseum* (Papaveraceae).

Preininger, V. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 124 (*uv, pmr, struct, bibl*)

Alkaloid PP1† **A-585**

$C_{19}H_{15}NO_5$ 337.331

Struct. unknown. Quaternary phenolic protoberberine. Minor alkaloid from *Papaver pavoninum* (Papaveraceae). Orange needles (MeOH) (as iodide). Mp 250° dec. (iodide). λ_{max} 222 ; 239 ; 251 ; 272 ; 352 (sh) ; 360 ; 468 (MeOH).

Táborská, E. *et al., Coll. Czech. Chem. Comm.*, 1988, **53**, 1845 (*isol, uv, ir, ms*)

Alkaloid PP1†, 9CI **A-586**

[158827-53-3]

$C_{17}H_{19}NO_3$ 285.342

Struct. unknown, prob. a normorphinane. Alkaloid from *Papaver pinnatifidium* (Papaveraceae). Mp 179°. Laevorotatory.

Slavík, J. *et al., Coll. Czech. Chem. Comm.*, 1994, **59**, 1879-1883 (*isol*)

***C*-Alkaloid Q** **A-587**

$C_{22}H_{27}N_3O_3$ 381.474

Minimum formula. Struct. unknown. Alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). Mp 276-283° dec. No col. with $Ce(SO_4)_2$.

Meyer, H. *et al., Helv. Chim. Acta*, 1956, **39**, 1208-1213 (*isol, uv*)

***Mucuna pruriens* Alkaloid Q** **A-588**

Mucuna pruriens *Base Q*

Struct. unknown. Alkaloid from *Mucuna pruriens* (Fabaceae). Bp 220-221°.

Picrate: Mp 152-154°.

Rakhit, S. *et al., Indian J. Pharm.*, 1956, **18**, 285; *CA*, **52**, 5748e (*isol*)

***Veratrum* Alkaloid Q** **A-589**

$C_{32}H_{53}NO_4$ 515.775

Steroidal alkaloid. Struct. unknown. Alkaloid from *Veratrum californicum* (Liliaceae). Mp 209-210°. $[\alpha]_D^{25}$ -95 ($CHCl_3$).

Keeler, R.F. *et al., Phytochemistry*, 1968, 303 (*isol*)

***C*-Alkaloid R** **A-590**

$C_{21}H_{27}N_2O_2^{\oplus}$ 339.456

Minimum formula. Struct. unknown. Quaternary alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). Violet col. with $Ce(SO_4)_2$. UV suggests indoline chromophore resembling *C*-Alkaloid B, A-400, *C*-Alkaloid C, A-436 and *C*-Alkaloid D, A-476.

Chloride: Mp 312° dec.

Perchlorate: Mp 317° dec.

Meyer, H. *et al., Helv. Chim. Acta*, 1956, **39**, 1208-1213 (*isol, uv*)

***Fritillaria imperialis* Alkaloid R** **A-591**

Fritillaria *Base R*

Prob. a steroidal alkaloid. Struct. unknown. Alkaloid from *Fritillaria imperialis* var. *lutea* (Liliaceae). Mp 134-136° Mp 213-215° (double Mp). Co-occurs with Imperonine, I-53.

Hydroiodide: Mp 205-207°.

Perchlorate: Mp 193-196°.

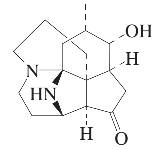
Methiodide: Mp 269° dec.

Paul, L. *et al., Chem. Ber.*, 1958, **91**, 1968

***Lycopodium fawcwttii* Alkaloid R** **A-592**

Lycopodium *Base R*

[53938-16-2]



Absolute Configuration

$C_{16}H_{24}N_2O_2$ 276.378

Alkaloid from *Lycopodium fawcettii* (Lycopodiaceae). Mp 129-130°. $[\alpha]_D$ +104.

Perchlorate: Mp 198-199°.

Burnell, R.H. *et al., Can. J. Chem.*, 1963, **41**, 3091 (*isol, ir*)

Burnell, R.H. *et al., Chem. Comm.*, 1974, 391 (*cryst struct*)

***Mucuna pruriens* Alkaloid R** **A-593**

Mucuna pruriens *Base R*

$C_{23}H_{35}NO_4$ 389.534

Struct. unknown. Alkaloid from *Mucuna pruriens* (Fabaceae). Bp 320°.

Oxalate: Mp 130-131° dec.

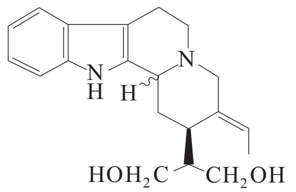
Picrate: Mp 172-173°.

Methiodide: Mp 95-96°.

Rakhit, S. *et al., Indian J. Pharm.*, 1956, **18**, 285; *CA*, **52**, 5748e (*isol*)

Alkaloid RMB 10 **A-594**

[71635-30-8]



$C_{20}H_{26}N_2O_2$ 326.438

Alkaloid from the stem bark of *Rauwolfia mombasiana* (Apocynaceae). Yellow amorph. powder.

Iwu, M.M. *et al., Planta Med.*, 1979, **36**, 208 (*isol, uv, ir, ms, struct*)

***Voacanga schweinfurthii* Alkaloid S_2** **A-595**

Struct. unknown. Bisindole alkaloid (*Aspidosperma-Aspidosperma* type). Alkaloid from the leaves of *Voacanga schweinfurthii* (Apocynaceae). Mol. formula not reported.

Newcombe, F. *et al., Planta Med.*, 1969, **17**, 276-280 (*isol, uv*)

Cordell, G.A. *et al., Alkaloids (Academic Press)*, 1981, **20**, 1; 266 (*rev*)

***Voacanga schweinfurthii* Alkaloid S_3** **A-596**

Struct. unknown. Bisindole alkaloid (*Aspidosperma-Aspidosperma* type). Alkaloid from the leaves of *Voacanga schweinfurthii* (Apocynaceae). Mol. formula not reported.

Newcombe, F. *et al., Planta Med.*, 1969, **17**, 276-280 (*isol, uv*)
Cordell, G.A. *et al., Alkaloids (Academic Press)*, 1981, **20**, 1; 266 (*rev*)

C-Alkaloid S A-597

$C_{19}H_{22}N_2$ 278.396

Approx. minimum formula. Struct. unknown. Alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). Mp 250° (as picrate). Red-violet col. with $Ce(SO_4)_2$ becoming colourless on standing. Tertiary base.

Meyer, H. *et al., Helv. Chim. Acta*, 1956, **39**, 1208-1213 (*isol, uv*)

Mucuna pruriens Alkaloid S A-598

Mucuna pruriens *Base S*
Struct. unknown. Alkaloid from *Mucuna pruriens* (Fabaceae). Bp 320°.

Picrate: Mp 165-166°.

Rakhit, S. *et al., Indian J. Pharm.*, 1956, **18**, 285; *CA*, **52**, 5748e (*isol*)

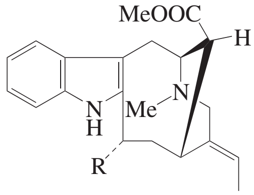
Alkaloid S-F A-599

$C_{15}H_{21}NO_3$ 263.336

Pyrrolizidine alkaloid. Struct. unknown. Alkaloid from *Senecio viscosus* dried plants (Asteraceae). Mp 228-230° dec. $[\alpha]_D^{22}$ -148 (c, 0.573 in $CHCl_3$).

Šantavý, F. *et al., Coll. Czech. Chem. Comm.*, 1962, **27**, 1666-1671

Alkaloid TC-D A-600



R = $C_2H_6NO_2$

$C_{23}H_{31}N_3O_4$ 413.516

Similar to Pagisulfine, P-11. Minor alkaloid from the root bark of *Tabernaemontana chippii* (Apocynaceae).

van Beek, T.A. *et al., J. Nat. Prod.*, 1985, **48**, 400-423 (*isol, uv, pmr, cmr, ms*)
Saxton, J.E. *et al., Nat. Prod. Rep.*, 1987, **4**, 591 (*rev, struct*)

Veratrum Alkaloid U A-601

$C_{36}H_{55}NO_{13}$ 709.829

Steroidal alkaloid, poss. an ester of Protoverine. Struct. unknown. Alkaloid from *Veratrum lobelianum* (Liliaceae). Mp 181-183°. $[\alpha]_D$ +7.6 ($CHCl_3$).

Bondarenko, N.V. *et al., Zh. Obshch. Khim.*, 1967, **37**, 332; *J. Gen. Chem. USSR (Engl. Transl.)*, 1967, **37**, 310 (*isol*)

C-Alkaloid UB A-602

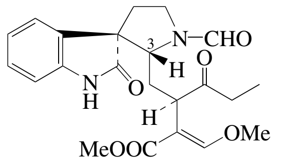
$C_{19}H_{23}N_2O_3^{\oplus}$ 327.402

Minimum formula. Struct. unknown. Alkaloid from calabash curare (*Strychnos* spp.) (Loganiaceae). Mp 238-240° dec. (as picrate). Carmine col. with $Ce(SO_4)_2$, becoming brown on standing.

Schmid, H. *et al., Helv. Chim. Acta*, 1947, **30**, 2081-2091; 1952, **35**, 1846-1879 (*isol, uv*)

Alkaloid Us 7 A-603

Us 7
[188790-08-1]



$C_{22}H_{26}N_2O_6$ 414.457
Alkaloid from *Uncaria attenuata*. Pale yellow oil. $[\alpha]_D^{25}$ -12.9 (c, 1.10 in MeOH). λ_{max} 208 ; 244 (MeOH).

3-Epimer: ***Alkaloid Us 8***. *Us 8*
[188790-09-2]
$C_{22}H_{26}N_2O_6$ 414.457
From *Uncaria attenuata*. Yellow oil. $[\alpha]_D^{25}$ -9.6 (c, 1.25 in MeOH). λ_{max} 208 ; 244 (MeOH).

Aimi, N. *et al., J.C.S. Perkin 1*, 1997, 187 (*isol, uv, pmr, cmr, struct*)

Gentiana Alkaloid VI A-604

$C_{16}H_{18}N_2O_3$ 286.33

Struct. unknown. Monoterpene alkaloid. Alkaloid from *Gentiana asclepiadea, Gentiana bulgarica* and *Gentiana cruciata* (Gentianaceae). Mp 248-252°.

Mollov, N.M. *et al., Dokl. Bulg. Akad. Nauk*, 1965, **18**, 947-949; *CA*, **64**, 10084h (*isol, ir*)
Cordell, G.A. *et al., Alkaloids (Academic Press)*, 1977, **16**, 431 (*rev*)

Lycopodium annotinum Alkaloid VI A-605

Lycopodium *Base VI*

$C_{16}H_{23}NO_2$ 261.363

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae).

Methiodide: Mp 294°. $[\alpha]_D^{20}$ -13.9.

Methochloride: Mp 263°.

Methoperchlorate: Mp 287.5°.

Methopicrate: Mp 163°.

Achmatowicz, O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1958, **32**, 485 (*isol, uv*)

Lycopodium annotinum Alkaloid VII A-606

Lycopodium *Base VII*

$C_{20}H_{29}NO_4$ 347.453

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae).

Methiodide: Mp 292°. $[\alpha]_D^{20}$ -11.1.

Methochloride: Mp 261°.

Methoperchlorate: Mp 295°.

Achmatowicz, O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1958, **32**, 485 (*isol, uv*)

Pachysandra terminalis Alkaloid VI A-607

Pachysandra *Base VI*
Steroidal alkaloid. Struct. unknown. Isol. from *Pachysandra terminalis* (Buxaceae). Mp 290-295°.

Kikuchi, T. *et al., Tet. Lett.*, 1964, 1817
Kikuchi, T. *et al., Yakugaku Zasshi*, 1967, **87**, 215; *CA*, **67**, 32888v

Rhodophiala bifida Alkaloid VI A-608

Rhodophiala *Base VI*

$C_{16}H_{17}NO_4$ 287.315

Amaryllidaceae alkaloid. Struct. unknown. Isol. from the bulbs of *Rhodophiala bifida* (Amaryllidaceae). Mp 272-273°. $[\alpha]_D^{25}$ -74 (MeOH).

Di-O-Ac: Mp 163-165°.

Dihydro: Mp 271°.

Wildman, W.C. *et al., Pharmazie*, 1967, **22**, 725; *CA*, **69**, 19337m (*isol*)

Lycopodium annotinum Alkaloid VIII A-609

Lycopodium *Base VIII*

$C_{16}H_{21}NO_3$ 275.347

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae).

Methiodide: Mp 216-217°.

Methochloride: Mp 255°.

Methoperchlorate: Mp 234-236°.

Methopicrate: Mp 134-136°.

Achmatowicz, O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1958, **32**, 485 (*isol, uv*)

Lycopodium annotinum Alkaloid XI A-610

Lycopodium *Base XI*

$C_{18}H_{25}NO_3$ 303.4

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae).

Methiodide: Mp 272°. $[\alpha]_D^{20}$ -95.8.

Methochloride: Mp 250°.

Methoperchlorate: Mp 267-268°.

Achmatowicz, O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1958, **32**, 485 (*isol, uv*)

Lycopodium annotinum Alkaloid XII A-611

Lycopodium *Base XII*

$C_{18}H_{25}NO_4$ 319.4

Struct. unknown. Alkaloid from *Lycopodium annotinum* (Lycopodiaceae).

Methiodide: Mp 283°. $[\alpha]_D^{20}$ -168.8.

Methochloride: Mp 270°.

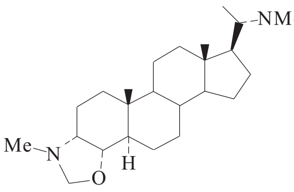
Methyl perchlorate: Mp 259-260°.

Methopicrate: Mp 219°.

Achmatowicz, O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1958, **32**, 485 (*isol, uv*)

Pachysandra terminalis Alkaloid XI A-612

*20-(Dimethylamino)-2′,3,3′,4-tetrahydro-3′-methylpregn-3-eno[3,4-*d*]oxazole, 8CI*
[15027-86-8]



$C_{25}H_{44}N_2O$ 388.635
Alkaloid from *Pachysandra terminalis* (Buxaceae) after hydrol. Mp 201-202°. $[\alpha]_D$ -60 ($CHCl_3$). Could be an artifact.

Kikuchi, T. *et al., Tet. Lett.*, 1964, 1817-1823 (*isol*)

Rhodophiala bifida Alkaloid XIII A-613

Rhodophiala *Base XIII*

$C_{16}H_{17}NO_4$ 287.315

Amaryllidaceae alkaloid. Struct. unknown. Isol. from the bulbs of *Rhodophiala bifida* (Amaryllidaceae). Mp 248-250°. $[\alpha]_D^{21}$ +12 (MeOH).

Wildman, W.C. *et al., Pharmazie*, 1967, **22**, 725; *CA*, **69**, 19337m (*isol*)

Pachysandra terminalis Alkaloid XVI A-614

Pachysandra *Base XVI*
Steroidal alkaloid. Struct unknown. Alkaloid from *Pachysandra terminalis* (Buxaceae). Mp 272-276°.

Kikuchi, T. *et al., Tet. Lett.*, 1964, 1817
Kikuchi, T. *et al., Yakugaku Zasshi*, 1967, **87**, 215; *CA*, **67**, 32888v

Rhodophiala bifida Alkaloid XXV A-615

Rhodophiala *Base XXV*

$C_{20}H_{23}NO_5$ 357.405

Amaryllidaceae alkaloid. Struct. unknown. Isol. from the bulbs of *Rhodophiala bifida* (Amaryllidaceae). Mp 204-206°. $[\alpha]_D^{21}$ -65 (MeOH).

Wildman, W.C. *et al., Pharmazie*, 1967, **22**, 725; *CA*, **69**, 19337m (*isol*)

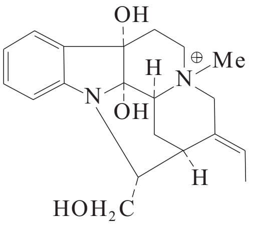
Pachysandra terminalis Alkaloid XXVII A-616

Pachysandra *Base XXVII*
Steroidal alkaloid. Struct. unknown. Alkaloid from *Pachysandra terminalis* (Buxaceae).

Kikuchi, T. *et al., Yakugaku Zasshi*, 1967, **87**, 215; *CA*, **67**, 32888v

C-Alkaloid Y A-617

C-Profluorocurine. 2,7-Dihydroxymavacurine
[6822-67-9]



$C_{20}H_{27}N_2O_3^{\oplus}$ 343.445
Quaternary alkaloid from *Strychnos guianensis*, *Strychnos toxifera* and calabash curare (*Strychnos* spp.) (Loganiaceae). Cryst. (as chloride). Red-violet colour with Ce(IV) becoming olive-green on standing.

17-Carboxylic acid, N*-de-Me, Me ester:* ***2,7-Dihydro-2,7-dihydroxypleiocarpamine****. 2,7-Dihydroxypleiocarpamine*
[87614-66-2]

$C_{20}H_{24}N_2O_4$ 356.421
Alkaloid from *Alstonia plumosa* (Apocynaceae). Cryst. (Me_2CO). Mp 152-158°. $[\alpha]_D$ +66 (c, 0.5 in MeOH). Called 2,7-Dihydroxypleiocarpamine in the lit., which is not strictly correct. No stereochem. assigned. CAS no. not found 8-14 CI.

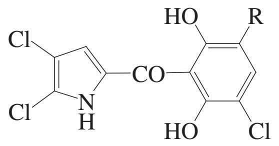
Asmis, H. *et al., Helv. Chim. Acta*, 1954, **37**, 1968-1973 (*isol, uv*)
Fritz, H. *et al., Annalen*, 1958, **611**, 268-276 (*uv*)
Hesse, M. *et al., Helv. Chim. Acta*, 1964, **47**, 878-911 (*struct*)
Jacquier, M.J. *et al., Phytochemistry*, 1982, **21**, 2973 (*2,7-Dihydroxypleiocarpamine*)
Penelle, J. *et al., Phytochemistry*, 2000, **53**, 1057-1066 (*isol, ir*)

Alkaloid YC2 A-618

Struct. unknown. Alkaloid from *Peganum harmala* (Zygophyllaceae). Characterised mainly by colour reactions and chem. props.

McKenzie, E. *et al., Phytochemistry*, 1975, **14**, 273-275 (*isol, uv*)

2-(3-Alkyl-5-chloro-2,6-dihydroxybenzoyl)-4,5-dichloro-1*H*-pyrroles A-619



2-(3-Chloro-5-hexyl-2,6-dihydroxybenzoyl)-4,5-dichloro-1*H*-pyrrole [188988-62-7]

$C_{17}H_{18}Cl_3NO_3$ 390.692
Prod. by *Streptomyces* sp. PA48424. GABA receptor antagonist, antibacterial agent. Yellow cryst. Sol. $CHCl_3$, EtOAc, MeOH; poorly sol. H_2O. Mp 145-147°. λ_{max} 225 ; 310 (ϵ 10000); 358 (ϵ 10700) (MeOH) (Berdy). λ_{max} 260 (ϵ 5200); 310 (ϵ 15000); 340 (MeOH/HCl) (Berdy). λ_{max} 233 ; 280 (ϵ 6400); 369 (ϵ 21300) (MeOH/NaOH) (Berdy).

2-[3-Chloro-2,6-dihydroxy-5-(4-methylpentyl)benzoyl]-4,5-dichloro-1*H*-pyrrole
[188988-63-8]

$C_{17}H_{18}Cl_3NO_3$ 390.692
Prod. by *Streptomyces* sp. PA48424. GABA receptor antagonist, antibacterial agent. Yellow cryst. Sol. $CHCl_3$, EtOAc, MeOH; poorly sol. H_2O. λ_{max} 255 ; 310 (ϵ 10400); 358 (ϵ 10300) (MeOH) (Berdy). λ_{max} 260 (ϵ 5300); 310 (ϵ 14900); 340 (MeOH/HCl) (Berdy).

2-[3-Chloro-2,6-dihydroxy-3-(4-methylhexyl)benzoyl]-4,5-dichloro-1*H*-pyrrole
[189008-36-4]

$C_{18}H_{20}Cl_3NO_3$ 404.719
Prod. by *Streptomyces* sp. PA48424. GABA receptor antagonist, antibacterial agent. Yellow cryst. Sol. $CHCl_3$, MeOH, EtOAc; poorly sol. H_2O. λ_{max} 225 ; 310 (ϵ 9300); 358 (ϵ 10000) (MeOH) (Berdy). λ_{max} 260 (ϵ 4800); 310 (ϵ 14100) (MeOH/HCl) (Berdy). λ_{max} 279 (ϵ 6100); 370 (ϵ 16000) (MeOH/NaOH) (Berdy).

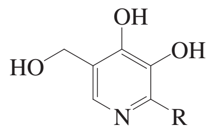
2-[3-Chloro-2,6-dihydroxy-5-(5-methylhexyl)benzoyl]-4,5-dichloro-1*H*-pyrrole
[188988-64-9]

$C_{18}H_{20}Cl_3NO_3$ 404.719
Prod. by *Streptomyces* sp. PA48424. GABA receptor antagonist, antibacterial agent. Yellow cryst. Sol. $CHCl_3$, MeOH, EtOAc; poorly sol. H_2O. λ_{max} 225 ; 310 (ϵ 9800); 357 (ϵ 4800) (MeOH) (Berdy). λ_{max} 258 (ϵ 4900); 310 (ϵ 14200) (MeOH/HCl) (Berdy). λ_{max} 233 ; 281 (ϵ 6100); 371 (ϵ 19700) (MeOH/NaOH) (Berdy).

Japan. Pat., 1997, 97 59 249; *CA*, **126**, 276425v

2-Alkyl-3,4-dihydroxy-5-hydroxymethylpyridines A-620

2-Alkyl-5-hydroxymethyl-3,4-pyridinediols



3,4-Dihydroxy-5-hydroxymethyl-2-propylpyridine
5-Hydroxymethyl-2-propyl-3,4-pyridinediol

$C_9H_{13}NO_3$ 183.207
Prod. by *Streptomyces* sp. GW23/1540.

3,4-Dihydroxy-5-hydroxymethyl-2-isopropylpyridine
5-Hydroxymethyl-2-(1-methylethyl)-3,4-pyridinediol

$C_9H_{13}NO_3$ 183.207
Prod. by *Streptomyces* sp. GW23/1540.

3,4-Dihydroxy-5-hydroxymethyl-2-(1-methylpropyl)pyridine
*5-Hydroxymethyl-2-(1-methylpropyl)-3,4-pyridinediol. 2-*sec*-Butyl-3,4-dihydroxy-5-hydroxymethylpyridine*

$C_{10}H_{15}NO_3$ 197.233
Prod. by *Streptomyces* sp. GW63/1571.

3,4-Dihydroxy-5-hydroxymethyl-2-(2-methylpropyl)pyridine
5-Hydroxymethyl-2-(2-methylpropyl)-3,4-pyridinediol. 3,4-Dihydroxy-5-hydroxymethyl-2-isobutylpyridine

$C_{10}H_{15}NO_3$ 197.233
Prod. by *Streptomyces* sp. GW23/1540.

Maskey, R.P. *et al., Z. Naturforsch., B*, 2005, **60**, 63-66 (*isol, pmr, cmr, ms*)

2-Alkyl-3,4-dihydroxyquinolines A-621

*2-Alkyl-3-hydroxy-4(1*H*)-quinolinones. 2-Alkyl-3,4-quinolinediols*

Metabs. of *Pseudomonas aeruginosa*. Signalling compds. involved in cell-to-cell signalling.

3,4-Dihydroxy-2-pentylquinoline
*2-Pentyl-3,4-quinolinediol, 9CI. 3-Hydroxy-2-pentyl-4(1*H*)-quinolinone*
[521313-34-8]
$C_{14}H_{17}NO_2$ 231.294

2-Hexyl-3,4-dihydroxyquinoline
*2-Hexyl-3,4-quinolinediol. 2-Hexyl-3-hydroxy-4(1*H*)-quinolinone*
[678172-89-9]
$C_{15}H_{19}NO_2$ 245.321

2-Heptyl-3,4-dihydroxyquinoline
*2-Heptyl-3,4-quinolinediol, 9CI. 2-Heptyl-3-hydroxy-4(1*H*)-quinolinone. PQS*
[521313-35-9]
$C_{16}H_{21}NO_2$ 259.347

3,4-Dihydroxy-2-octylquinoline
*2-Octyl-3,4-quinolinediol. 3-Hydroxy-2-octyl-4(1*H*)-quinolinone*
[678172-90-2]
$C_{17}H_{23}NO_2$ 273.374

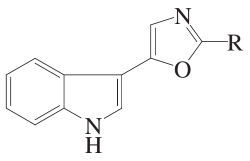
3,4-Dihydroxy-2-nonylquinoline
*2-Nonyl-3,4-quinolinediol, 9CI. 3-Hydroxy-2-nonyl-4(1*H*)-quinolinone*
[521313-36-0]
$C_{18}H_{25}NO_2$ 287.401

3,4-Dihydroxy-2-undecylquinoline
*2-Undecyl-3,4-quinolinediol, 9CI. 3-Hydroxy-2-undecyl-4(1*H*)-quinolinone*
[678172-91-3]
$C_{20}H_{29}NO_2$ 315.455

Takeda, R. *et al., CA*, 1960, **54**, 16533i (*isol*)
Pesci, E.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1999, **96**, 11229-11234 (*heptyl, isol, synth, pmr, cmr*)
Lepine, F. *et al., Biochim. Biophys. Acta*, 2003, **1622**, 36-41 (*detn*)
Deziel, E. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2004, **101**, 1339-1344 (*occur, biosynth, ms*)
Bredenbruch, F. *et al., J. Bacteriol.*, 2005, **187**, 3630-3635 (*biosynth*)

3-(2-Alkyl-5-oxazolyl)-1*H*-indoles A-622

*2-Alkyl-5-(1*H*-indol-3-yl)oxazole*



Revised structs. (1999) for several members of this series which were formerly descr. as pyrazoloisoquinolines.

3-(2-Methyl-5-oxazolyl)-1*H*-indole, 9CI
5-(3-Indolyl)-2-methyloxazole. ***Pimprinine****. WS 30581C. Antibiotic WS 30581C. APHE 3*
[13640-26-1]
[179728-23-5]
$C_{12}H_{10}N_2O$ 198.224
Metab. of *Streptomyces pimprina*, *Streptoverticillium griseocarneum* and *Streptoverticillium olivoreticuli*. Monoamine oxidase inhibitor. Shows antiepileptic effects. Prisms (C_6H_6), needles. Mp 204-205°. λ_{max} 224 (ε 24600); 266 (ε 15500); 282 (sh) (ε 12100); 298 (sh) (ε 11000) (EtOH) (Derep).

3-(2-Ethyl-5-oxazolyl)-1*H*-indole, 9CI
2-Ethyl-5-(3-indolyl)oxazole. ***Pimprinethine****. APHE 1*
[73053-81-3]
[146426-35-9]
$C_{13}H_{12}N_2O$ 212.251
Metab. of *Streptoverticillium olivoreticuli*, *Streptoverticillium griseocarneum* and *Streptomyces cinnamomeus*. Cryst. (C_6H_6 or $CHCl_3$). Mp 163-165° (161-163°).

3-(2-Propyl-5-oxazolyl)-1*H*-indole
5-(3-Indolyl)-2-propyloxazole. ***Antibiotic WS 30581A****. APHE 2. WS 30581A*
[93773-64-9]
[146426-36-0]
$C_{14}H_{14}N_2O$ 226.277
Prod. by *Streptoverticillium waksmanii* and *Streptoverticillium griseocarneum*. Antiplatelet, cytotoxic and antithrombotic agent. Needles. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 128-130°. λ_{max} 224 (ε 24000); 266 (ε 15400); 282 (sh) (ε 13000); 298 (sh) (ε 11200) (EtOH) (Derep).
▶ LD_{50} (mus, ipr) 250-750 mg/kg.

3-(2-Butyl-5-oxazolyl)-1*H*-indole, 9CI
2-Butyl-5-(3-indolyl)oxazole. ***Antibiotic WS 30581B****. APHE 4. WS 30581B*
[93773-63-8]
[179728-24-6]
$C_{15}H_{16}N_2O$ 240.304
Prod. by *Streptoverticillium waksmanii* and *Streptoverticillium griseocarneum*. Platelet aggregation inhibitor. An antithrombotic agent. Needles (C_6H_6/hexane). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 123-125°. λ_{max} 224 (ε 24000); 266 (ε 15400); 282 (sh) (ε 13000); 298 (sh) (ε 11200) (EtOH) (Derep).

3-[2-(2-Methylpropyl)-5-oxazolyl]-1*H*-indole
5-(3-Indolyl)-2-isobutyloxazole. ***Labradorin 1***
[477951-20-5]
$C_{15}H_{16}N_2O$ 240.304
Prod. by *Pseudomonas syringae* pv. *coronafaciens*. Cytotoxic. Prisms (Me_2CO). Mp 147-148°.

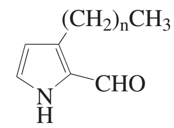
3-(2-Pentyl-5-oxazolyl)-1*H*-indole
5-(3-Indolyl)-2-pentyloxazole. ***Labradorin 2***
[326494-56-8]
$C_{16}H_{18}N_2O$ 254.331
Prod. by *Pseudomonas syringae* pv. *coronafaciens*. Cytotoxic. Small plates (MeOH). Mp 130-132°.

3-(2-Benzyl-5-oxazolyl)-1*H*-indole, 9CI
*3-[2-(Phenylmethyl)-5-oxazolyl]-1*H*-indole. 2-Benzyl-5-(3-indolyl)oxazole.* ***Pimprinaphine***
[73053-85-7]
$C_{18}H_{14}N_2O$ 274.321
Metab. of *Streptoverticillium olivoreticuli*. Cryst. (C_6H_6). Mp 200-201° (198-200°).

Bhate, D.S. *et al., Experientia*, 1960, **16**, 504 (*Pimprinine, isol*)
Joshi, B.S. *et al., Tetrahedron*, 1963, **19**, 1437-1439 (*Pimprinine, uv, ir, struct, synth*)
Oikawa, Y. *et al., Heterocycles*, 1979, **12**, 1457-1462 (*synth*)
Koyama, Y. *et al., Agric. Biol. Chem.*, 1981, **45**, 1285-1287 (*Pimprinine, Pimprinethine, Pimprinaphine, isol, uv, pmr, synth*)
Yoshioka, T. *et al., J. Chem. Res., Synop.*, 1981, 194-195; *J. Chem. Res., Miniprint*, 2252-2281 (*synth, uv, ir, pmr, ms*)
Noltemeyer, M. *et al., J. Antibiot.*, 1982, **35**, 549-555 (*Pimprinethine, isol, uv, ir, pmr, cmr, ms, cryst struct*)
Umehara, K. *et al., J. Antibiot.*, 1984, **37**, 1153-1160 (*WS 30581*)
Somei, M. *et al., Heterocycles*, 1985, **23**, 1101-1106 (*synth*)
Doyle, K.J. *et al., Synthesis*, 1994, 1021-1022 (*synth, ir, pmr, cmr*)
Kelly, T.R. *et al., Tet. Lett.*, 1999, **40**, 1857-1860 (*APHE 1-4*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2002, **65**, 1793-1797 (*Labradorins, cryst struct*)
Kumar, D. *et al., Tet. Lett.*, 2008, **49**, 867-869 (*synth*)

3-Alkyl-1*H*-pyrrole-2-carboxaldehydes A-623

3-Alkyl-2-formylpyrroles



Isol. as a mixt. of 3.3% n = 18, 12.5% n = 19, 49% n = 20, 25% n = 21, and 10.2% n = 22. The substitution pattern of these constits. has been questioned (Stierle *et al*). Metabs. of the marine sponge *Oscarella lobularis.*

3-Nonadecyl-1*H*-pyrrole-2-carboxaldehyde
[57992-51-5]
$C_{24}H_{43}NO$ 361.61
n = 18.

3-Eicosyl-1*H*-pyrrole-2-carboxaldehyde
*3-Icosyl-1*H*-pyrrole-2-carboxaldehyde*
[57992-52-6]
$C_{25}H_{45}NO$ 375.637
n = 19.

3-Heneicosyl-1*H*-pyrrole-2-carboxaldehyde
[57992-53-7]
$C_{26}H_{47}NO$ 389.663
n = 20.

*12′,13′-Didehydro(*E*-): 13-(12-Heneicosenyl)-1*H*-pyrrole-2-carboxaldehyde, 9CI*
[57992-57-1]
$C_{26}H_{45}NO$ 387.648
Isol. from the marine sponge *Oscarella lobularis.*

3-Docosyl-1*H*-pyrrole-2-carboxaldehyde
[57992-54-8]
$C_{27}H_{49}NO$ 403.69
n = 21.

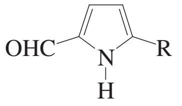
3-Tricosyl-1*H*-pyrrole-2-carboxaldehyde
[57992-55-9]

$C_{28}H_{51}NO$ 417.717
n = 22.

Cimino, G. *et al., Experientia*, 1975, **31**, 1387-1389 (*isol, uv, ir, pmr, ms, struct*)
Stierle, D.B. *et al., J.O.C.*, 1980, **45**, 4980-4982 (*struct*)

5-Alkyl-1*H*-pyrrole-2-carboxaldehydes A-624

2-Alkyl-5-formylpyrroles



5-Nonyl-1*H*-pyrrole-2-carboxaldehyde
[89631-84-5]

$C_{14}H_{23}NO$ 221.342
Isol. from a soft coral, *Telesto* sp., and its associated, but unidentified, demosponge. Yellow oil. Not possible to identify the exact source of the natural product since it perfused both organisms.

5-Pentadecyl-1*H*-pyrrole-2-carboxaldehyde
[75233-97-5]

$C_{20}H_{35}NO$ 305.503
Metab. from a marine sponge *Laxosuberites* sp. Isol. in admixture (46%) with the hexadecyl (12%), heptadecyl (23%) and nonadecyl (19%) homologues. λ_{max} 297 (ϵ 16000) (MeCN) (Derep).

*6′,7′*E*-Didehydro: 5-(6-Pentadecenyl)-1*H*-pyrrole-2-carboxaldehyde*
$C_{20}H_{33}NO$ 303.487
Metab. of the sponge *Mycale tenuispiculata*. Pale yellow solid. Mp 42-44°. λ_{max} 297 (ϵ 15400) (MeCN).

5-(13-Methyltetradecyl)-1*H*-pyrrole-2-carboxaldehyde [233744-63-3]

$C_{20}H_{35}NO$ 305.503
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-Hexadecyl-1*H*-pyrrole-2-carboxaldehyde
[75233-98-6]

$C_{21}H_{37}NO$ 319.529
Metab. from *Laxosuberites* sp. See note under pentadecyl above.

5-(14-Methylpentadecyl)-1*H*-pyrrole-2-carboxaldehyde [233744-64-4]

$C_{21}H_{37}NO$ 319.529
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-Heptadecyl-1*H*-pyrrole-2-carboxaldehyde
[75233-99-7]

$C_{22}H_{39}NO$ 333.556
Metab. from *Laxosuberites* sp. See note under pentadecyl above.

*9,10*Z*-Didehydro: 5-(9*Z*-Heptadecenyl)-1*H*-pyrrole-2-carboxaldehyde*
[233744-73-5]
$C_{22}H_{37}NO$ 331.54
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-Octadecyl-1*H*-pyrrole-2-carboxaldehyde
[262351-87-1]

$C_{23}H_{41}NO$ 347.583
Isol. from *Mycale mytilorum*. Pale yellow flakes. Mp 56-58°. λ_{max} 302 (ϵ 16000) (EtOH).

5-(16-Methylheptadecyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 6
[705973-02-0]

$C_{23}H_{41}NO$ 347.583
Isol. from the sponge *Mycale cecilia*. Amorph. powder. λ_{max} 203 (ϵ 6260); 249 (ϵ 2080); 300 (ϵ 9790) (MeOH).

5-Nonadecyl-1*H*-pyrrole-2-carboxaldehyde
[75234-00-3]

$C_{24}H_{43}NO$ 361.61
Metab. from *Laxosuberites* sp. See note under pentadecyl above.

*9,10*Z*-Didehydro: 5-(9*Z*-Nonadecenyl)-1*H*-pyrrole-2-carboxaldehyde*
[233744-74-6]
$C_{24}H_{41}NO$ 359.594
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

*12,13*Z*-Didehydro: 5-(12*Z*-Nonadecenyl)-1*H*-pyrrole-2-carboxaldehyde.* ***Mycalazal 4***
[705972-97-0]
$C_{24}H_{41}NO$ 359.594
Isol. from the sponge *Mycale cecilia*. Amorph. powder. λ_{max} 202 (ϵ 7585); 249 (ϵ 2340); 300 (ϵ 11760) (MeOH).

5-Eicosyl-1*H*-pyrrole-2-carboxaldehyde
[233744-67-7]

$C_{25}H_{45}NO$ 375.637
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-(9*Z*-Heneicosenyl)-1*H*-pyrrole-2-carboxaldehyde [233744-65-5]

$C_{26}H_{45}NO$ 387.648
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-(14*Z*-Heneicosenyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 8
[705973-25-7]
Isol. from the sponge *Mycale cecilia*. Amorph. powder. λ_{max} 202 (ϵ 7800); 248 (ϵ 2320); 300 (ϵ 11290) (MeOH).

5-(12*Z*,15*Z*-Heneicosadienyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 5
[705972-98-1]

$C_{26}H_{43}NO$ 385.632
Isol. from the sponge *Mycale cecilia*. Oil. λ_{max} 204 (ϵ 9250); 248 (ϵ 2390); 300 (ϵ 11150) (MeOH).

5-(12*Z*,15*Z*,18*Z*-Heneicosatrienyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 3
[705972-95-8]

$C_{26}H_{41}NO$ 383.616
Isol. from the sponge *Mycale cecilia*. Oil. λ_{max} 204 (ϵ 14690); 248 (ϵ 3440); 300 (ϵ 15400) (MeOH).

5-(12*Z*-Docosenyl)-1*H*-pyrrole-2-carboxaldehyde [233744-66-6]

$C_{27}H_{47}NO$ 401.674
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*. Indexed as the Δ^{11}-isomer in CAS.

5-Tricosyl-1*H*-pyrrole-2-carboxaldehyde
[233744-70-2]

$C_{28}H_{51}NO$ 417.717
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

*9,10*Z*-Didehydro: 5-(9*Z*-Tricosenyl)-1*H*-pyrrole-2-carboxaldehyde*
[233744-68-8]
$C_{28}H_{49}NO$ 415.701
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

*14,15*Z*-Didehydro: 5-(14*Z*-Tricosenyl)-1*H*-pyrrole-2-carboxaldehyde*
[233744-69-9]
$C_{28}H_{49}NO$ 415.701
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

*14,15*Z*,17,18*Z*-Tetradehydro: 5-(14*Z*,17*Z*-Tricosadienyl)-1*H*-pyrrole-2-carboxaldehyde.* ***Mycalazal 9***
[705973-27-9]
$C_{28}H_{47}NO$ 413.685
Isol. from the sponge *Mycale cecilia*. Oil. λ_{max} 201 (ϵ 14170); 248 (ϵ 4060); 300 (ϵ 21160) (MeOH).

*14,15*Z*,17,18*Z*,20,21*Z*-Hexadehydro: 5-(14*Z*,17*Z*,20*Z*-Tricosatrienyl)-1*H*-pyrrole-2-carboxaldehyde.* ***Mycalazal 7***
[705973-15-5]
$C_{28}H_{45}NO$ 411.67
Isol. from the sponge *Mycale cecilia*. Oil. λ_{max} 204 (ϵ 9250); 248 (ϵ 2390); 300 (ϵ 11150) (MeOH).

5-(11*Z*-Pentacosenyl)-1*H*-pyrrole-2-carboxaldehyde [233744-71-3]

$C_{30}H_{53}NO$ 443.755
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-(15*Z*-Pentacosenyl)-1*H*-pyrrole-2-carboxaldehyde [233744-72-4]

$C_{30}H_{53}NO$ 443.755
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-(16*Z*-Pentacosenyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 12
[705973-36-0]

$C_{30}H_{53}NO$ 443.755
Isol. from the sponge *Mycale cecilia*.

5-(18*Z*-Pentacosenyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 13
[705973-38-2]

$C_{30}H_{53}NO$ 443.755
Isol. form the sponge *Mycale cecilia*.

5-(16*Z*,19*Z*-Pentacosadienyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 11
[705973-35-9]
Isol. from the sponge *Mycale cecilia*. Oil. λ_{max} 202 (ϵ 6040); 248 (ϵ 1800); 301 (ϵ 7630) (MeOH).

5-(16*Z*,19*Z*,22*Z*-Pentacosatrienyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 10
[705973-28-0]
Isol. from the sponge *Mycale cecilia*. Oil. λ_{max} 204 (ϵ 11920); 248 (ϵ 3690); 300 (ϵ 16900) (MeOH).

5-(10*Z*,13*Z*,16*Z*,19*Z*,22*Z*-Pentacosapentaenyl)-1*H*-pyrrole-2-carboxaldehyde, 9CI
Mycalazal 2
[185389-83-7]

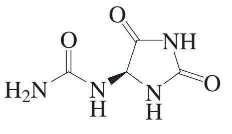
$C_{30}H_{45}NO$ 435.692
Metab. from *Mycale micracanthoxea*. Cytotoxic agent. Oil.

5-(7*Z*,10*Z*,13*Z*,16*Z*,19*Z*,22*Z*-Pentacosahexaenyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 1
[185389-71-3]
Metab. of the sponge *Mycale micracanthoxea*. Oil.

Stierle, D.B. *et al., J.O.C.*, 1980, **45**, 4980 (*isol, uv, ir, pmr, cmr, ms, struct*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1984, **37**, 227 (*isol, uv, ir, pmr, cmr, ms, struct, synth*)
Ortega, M.J. *et al., Tetrahedron*, 1997, **53**, 331-340; 2004, **60**, 2517-2524 (*Mycalazals 1-13*)
Compagnone, R.S. *et al., Nat. Prod. Lett.*, 1999, **13**, 203-211 (*alkenyls, branched-chain alkyls*)
Reddy, G.B.S. *et al., Bioorg. Med. Chem.*, 2000, **8**, 27-36 (*octadecyl*)
Venkatesham, U. *et al., J. Nat. Prod.*, 2000, **63**, 1318-1320 (*6-pentadecenyl*)
Hansen, T.V. *et al., Tet. Lett.*, 2004, **45**, 2809-2811 (*Mycalazal 2, synth*)

Allantoin, BAN, USAN A-625

(2,5-Dioxo-4-imidazolidinyl)urea, 9CI. 5-Ureido-2,4-imidazolidinedione. Glyoxylic diureide. 5-Ureidohydantoin. Dermalex. Cordianin. Actinac. Alphosyl



(*R*)-*form*

$C_4H_6N_4O_3$ 158.116

(±)-*form* [5377-33-3]
Occurs in allantoic fluid. A product of purine metabolism. V. widely distributed in biol. systems, isol. from numerous plants. Isol. from Bambusa oldhamii (green tomato), *Allophylus edulis* var *edulis*, *Allophylus edulis* var *gracilis*, *Strychnos cathayensis*, roots of *Pyrostegia venusta*, marine sponges *Cymbastela cantharella* and *Tedania digitala*, and cows milk. Formed in animals, except primates, by enzymic oxidn. of Uric acid, U-45. Antiinflammatory, antipsoriatic (disputed), topical vulnerary agent. Promotes wound healing. Monoclinic prisms (H_2O). V. spar. sol. H_2O; spar. sol. org. solvs. Mp 238-240° dec. Log P -1.54 (calc). Component of numerous prepns. Actinac, Alphosyl, Dermalex.

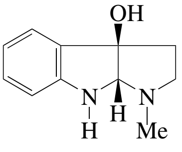
▶ YT1600000

[97-59-6 ((±)-*form*), 61504-48-1]

Org. Synth., Coll. Vol., 2, 1943, 21-23 (*synth, bibl*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 2569 (*occur*)
Mecca, S.B. *et al., Soap, Perfum. Cosmet.*, 1976, **49**, 434; 481; 483-485 (*rev*)
Coxon, B. *et al., J.O.C.*, 1977, **42**, 3132-3140 (*cmr*)
Mecca, S.B. *et al., Cosmet. Toiletries*, 1978, **93**, 39-41 (*rev*)
Cook, A.F. *et al., J.O.C.*, 1980, **45**, 4020-4025 (*isol*)
Chen, K.J. *et al., Taiwan Kexue*, 1989, **42**, 21-24; *CA*, **113**, 55816 (*(±)-form, isol*)
Hoffmann-Bohm, K. *et al., Planta Med.*, 1992, **58**, 544-548 (*(±)-form, isol*)
Mourabit, A.A. *et al., J. Nat. Prod.*, 1997, **60**, 290-291 (*(±)-form, isol*)
Shingfield, K.J. *et al., J. Chromatogr., B*, 1998, **706**, 342-346 (*hplc*)
Ferreira, D.T. *et al., Quim. Nova*, 2000, **23**, 42-46 (*isol*)

Alline A-626

*2,3,8,8*a*-Tetrahydro-1-methylpyrrolo[2,3-*b*]indol-3*a*(1*H*)-ol, 9CI*
[101053-34-3]



Relative Configuration

$C_{11}H_{14}N_2O$ 190.244
Alkaloid from Chinese chives (*Allium odorum*) and several other *Allium* spp. Mp 91-92°. $[\alpha]_D$ +136.3 (c, 1.218 in HCl). λ_{max} 245 (log ϵ 3.68); 303 (log ϵ 3.14) (no solvent reported).

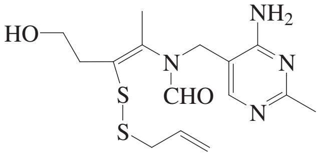
Hydrochloride: Mp 196-197°.

Me ether, N^8-*Me: 2,3,8,8*a*-Tetrahydro-3*a*-methoxy-1,8-dimethylpyrrolo[2,3-*b*]indole.* ***Alkaloid CPC 1***. *CPC 1*
$C_{13}H_{18}N_2O$ 218.298
Alkaloid from *Chimonanthus praecox* f. *concolor*. Amorph. solid. $[\alpha]_D^{26}$ -88 (c, 0.1 in MeOH). (3*aR*,8*aR*)-config. determined. λ_{max} 205 (log ϵ 4.15); 251 (log ϵ 3.72); 301 (log ϵ 3.14) (MeOH).

Tashkhodzhaev, B. *et al., Khim. Prir. Soedin.*, 1985, **21**, 687-691; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 645-649 (*isol, cryst struct, uv*)
Samikov, K. *et al., Khim. Prir. Soedin.*, 1986, **22**, 383; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 362 (*occur*)
Antsupova, T.P. *et al., Rastit. Resur.*, 1987, **23**, 436; *CA*, **107**, 214830x (*occur*)
Kitajima, M. *et al., Tet. Lett.*, 2006, **47**, 3199-3202 (*CPC1*)

Allithiamine A-627

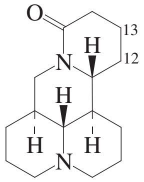
N-*[(4-Amino-2-methyl-5-pyrimidinyl)methyl]*-N-*[4-hydroxy-1-methyl-2-(2-propenyldithio)-1-butenyl]formamide, 9CI*
[554-44-9]



$C_{15}H_{22}N_4O_2S_2$ 354.496
Naturally-occurring open-chain thiamine analogue. Obt. from garlic (*Allium sativum*). Imparts meaty flavour to foods. Has vitamin B_1 activity. Investigated as a dietary supplement to enhance muscle performance and as treatment for thiamine deficiency. Cryst. (C_6H_6). Mp 132-133° dec.

Matsukawa, T. *et al., Science (Washington, D.C.)*, 1953, **118**, 325 (*isol, struct*)
Matsukawa, T. *et al., CA*, 1955, **49**, 7572g (*synth*)
Baker, H. *et al., J. Nutr. Sci. Vitaminol.*, Suppl., 1976, **22**, 63-68 (*pharmacol*)
Doyle, M.R. *et al., Int. J. Sport Nutr.*, 1997, **7**, 39-47 (*use*)

Allomatrine A-628



(+)-*form*

$C_{15}H_{24}N_2O$ 248.367
Stereoisomer of Matrine, M-121, Isomatrine, I-244, Sophoridine, S-380 and Darvasamine, D-79.

(+)-*form* [641-39-4]
Obt. by isomerisation of Matrine, M-121. Mp 103-105°. $[\alpha]_D^{25}$ +77.9. Incorr. stated by Ibragimov *et al* (1979) to have been isol. by Ueno *et al* from *Sophora flavescens.* This was Isomatrine.

*Methiodide:*Dec. at 315°.

Picrate: Mp 177°.

(-)-*form*
Leontine†. *Isoleontine*
[6783-60-4]
Alkaloid from *Leontice eversmannii* and *Leontice darvasica* (Leonticaceae). Mp 107-108°. Bp_3 175-190°. $[\alpha]_D$ -78.2 (EtOH). The original isolate of Leontine from *L. eversmannii* (Yunusov, 1949) was opt. inactive. It may have been the (±)-form, or a different alkaloid. Platonova *et al* (1953) isolated the (-)-form, which they called Isoleontine, but later workers used the name Leontine for the (-)-form.

Perchlorate: Mp 252°.

Methiodide: Mp 297°.

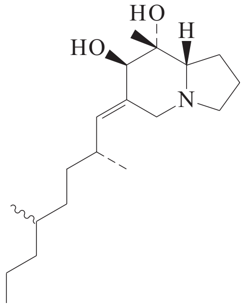
13-Oxo: ***Leontalbamine***
$C_{15}H_{22}N_2O_2$ 262.351
Alkaloid from *Leontice alberti*. Mp 195°. $[\alpha]_D$ -93. Struct. dubious. Given in the ref. as the unlikely 12,13-didehydro, 13-hydroxy enol tautomer. However struct. and MF do not agree in ref. CAS no. not found 8-14 CI. λ_{max} 220 (log ϵ 3.4) (no solvent reported).

(±)-*form*
Mp 85-87°.
Hydrochloride: Mp 215-217°.

Platonova, T.F. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1953, **23**, 921-926 (*Leontine*)
Bohlmann, F. *et al., Chem. Ber.*, 1958, **91**, 2176-2189 (*ir*)
Rulko, F. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1961, **31**, 282-285 (*Leontine*)
Mandell, L. *et al., J.A.C.S.*, 1965, **87**, 5234-5236 (*synth*)
Vul'fson, N.S. *et al., Khim. Geterotsikl. Soedin.*, 1974, 251-260; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1974, **10**, 221-229 (*ir*)
Bohlmann, F. *et al., Chem. Ber.*, 1975, **108**, 1043-1051 (*cmr*)
Ibragimov, B.T. *et al., Khim. Prir. Soedin.*, 1979, **15**, 416-417; *Chem. Nat. Compd. (Engl. Transl.)*, 368-369 (*cryst struct*)
Ibragimov, B.T. *et al., Khim. Prir. Soedin.*, 1982, **18**, 71-75; *Chem. Nat. Compd. (Engl. Transl.)*, 66-69 (*rev, stereochem*)
Shakirov, R. *et al., Khim. Prir. Soedin.*, 1996, **32**, 615-681; *Chem. Nat. Compd. (Engl. Transl.)*, 1996, **32**, 596-675 (*Leontalbamine*)

Allopumiliotoxin 309D A-629

6-(2,5-Dimethyloctylidene)octahydro-8-methyl-7,8-indolizinediol, 9CI
[141643-33-6]

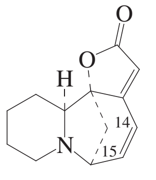


$C_{19}H_{35}NO_2$ 309.491
Alkaloid from skin extracts of the Panamanian poison frog *Dendrobates pumilio*.

Tokuyama, T. *et al., Tetrahedron*, 1991, **47**, 5415 (*isol, cmr, ms, struct*)

Allosecurinine A-630

Phyllochrysine. 2-Episecurinine. Viroallosecurinine



(-)-*form*

$C_{13}H_{15}NO_2$ 217.267
Viroallosecurinine is the (+)-enantiomer.

(-)-*form* [884-68-4]
Alkaloid from the leaves and roots of *Securinega suffruticosa*. Minor alkaloid from the roots of *Phyllanthus discoides*. Also isol. from bark and roots of *Margaritaria indica* (Euphorbiaceae). Yellow needles (Et_2O). Mp 136-138° (128°). $[\alpha]_D^{26}$ -1082 (EtOH). $[\alpha]_D$ -1140 ($CHCl_3$).
Hydrochloride:
Cubes (EtOH). Mp 248° dec. $[\alpha]_D^{30}$ -335 (EtOH).
Picrate:
Yellow needles (EtOH). Mp 231-232° dec.
14,15-Dihydro:
Needles (petrol). Mp 91°.
14,15-Dihydro, 15β-hydroxy: ***14,15-Dihydroallosecurinine-15-ol***
[119817-92-4]
$C_{13}H_{17}NO_3$ 235.282
Alkaloid from the leaves of *Phyllanthus discoides* (Euphorbiaceae). Orange-yellow cryst. (1-propanol). Mp 157-158°. $[\alpha]_D^{25}$ -96 (c, 0.48 in EtOH).
14,15-Dihydro, 15α-methoxy: ***14,15-Dihydro-15-methoxyphyllochrysine***. *15-Methoxy-14,15-dihydrophyllochrysine*
[128855-48-1]
$C_{14}H_{19}NO_3$ 249.309
Alkaloid from bark and roots of *Margaritaria indica* (Euphorbiaceae). Needles (petrol). Mp 141°. $[\alpha]_D$ +71 (c, 0.6 in MeOH).
14,15-Dihydro, 15α-methoxy, hydrobromide:
Plates (MeOH/Me_2CO). Mp 182-183°.

(+)-*form* [1857-30-3]
Alkaloid from the leaves of *Securinega virosa* (Euphorbiaceae). Yellow prisms (Me_2CO). Mp 136-138°. $[\alpha]_D^{20}$ +1084.6 (c, 0.05 in EtOH).
14,15-Dihydro, 15β-ethoxy: ***15β-Ethoxy-14,15-dihydroviroallosecurinine***
[936951-59-6]
$C_{15}H_{21}NO_3$ 263.336
Alkaloid from *Securinega suffruticosa*.

Parello, J. *et al., Bull. Soc. Chim. Fr.*, 1963, 898-910 (*uv, ir, pmr*)
Nakano, T. *et al., J.O.C.*, 1963, **28**, 2619-2621; 1964, **29**, 3441-3443 (*uv, ord, cd, conformn, abs config*)
Saito, S. *et al., Chem. Ind. (London)*, 1964, 1263-1264 (*struct, Viroallosecurinine*)
Bevan, C.W.L. *et al., Chem. Ind. (London)*, 1964, 2054 (*isol*)
Chatterjee, A. *et al., J. Indian Chem. Soc.*, 1964, **41**, 163-172 (*isol, ir, pmr, struct*)
Saito, S. *et al., Yakugaku Zasshi*, 1964, **84**, 1126; *CA*, **62**, 5498d (*isol, Viroallosecurinine*)
Mukherjee, R. *et al., Indian J. Chem.*, 1966, **4**, 459 (*isol, uv*)
Horii, Z. *et al., Chem. Pharm. Bull.*, 1970, **18**, 2009-2012 (*synth*)
Sankawa, U. *et al., Tet. Lett.*, 1974, 1867-1868 (*biosynth*)
Beutler, J.A. *et al., J. Nat. Prod.*, 1984, **47**, 677-681 (*cmr*)
Mensah, J.L. *et al., J. Nat. Prod.*, 1988, **51**, 1113-1115 (*14,15-Dihydroallosecurinine-15β-ol*)
Arbain, D. *et al., Aust. J. Chem.*, 1990, **43**, 439-445 (*15α-Methoxy-14,15-dihydrophyllochrysine, cryst struct, abs config*)
Honda, T. *et al., Tet. Lett.*, 2004, **45**, 5211-5213 (*synth*)
Wang, Y. *et al., Zhongguo Tianran Yaowu*, 2006, **4**, 260-263; *CA*, **146**, 518050b (*Ethoxydihydroviroallosecurinine*)
Yuan, W. *et al., Nat. Prod. Res.*, 2007, **21**, 234-242 (*isol, pmr, cmr*)
Bardaji, G.G. *et al., J.O.C.*, 2008, **73**, 7657-7662 (*synth*)

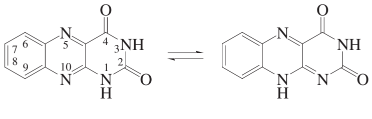
Allothiobinupharidine A-631

Struct. unknown
$C_{30}H_{42}N_2O_2S$ 494.74
Nuphar alkaloid. Alkaloid from the rhizomes of *Nuphar luteum* (Nymphaeaceae). Plates (as diperchlorate). Mp 320-325° (diperchlorate).

Achmatowicz, O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1962, **36**, 1815-1825 (*isol*)

Alloxazine A-632

*Benzo[g]pteridine-2,4(1*H*,3*H*)-dione, 9CI. 6,7-Benzolumazine*
[490-59-5]



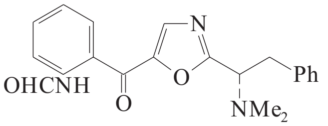
$C_{10}H_6N_4O_2$ 214.183
Parent compd. exists in 1*H*,3*H*-form. In the older lit., posns. 5,6,7,8,9,10 are often numbered 10,5,6,7,8,9 respectively. Greyish-green powder. V. spar. sol. EtOH; insol. H_2O, Et_2O. Mp 300° dec. The original synthesis of alloxazine (Kühling, 1891) prob. gave a material containing little of the desired product.

(3*H*,10*H*)-*form*
*Benzo[g]pteridine-2,4(3*H*,10*H*)-dione. Isoalloxazine. Flavin*
Parent residue present in Riboflavine. Many substd. derivs. synthesised. Same CAS no. as Alloxazine.
3,10-Di-Me: [4074-59-3]
$C_{12}H_{10}N_4O_2$ 242.237
Orange-yellow needles (AcOH). Mp 320-325° dec. Bitter taste.
10-Ph: [6851-14-5]
$C_{16}H_{10}N_4O_2$ 290.281
Orange-yellow prisms (AcOH). V. spar. sol. H_2O. Tasteless.
10-Ph, 3-Me: [35804-39-8]
$C_{17}H_{12}N_4O_2$ 304.307
Orange-yellow cryst. (AcOH). Stable on heating to at least 360°. Tasteless.
10-Benzyl: [21708-43-0]
$C_{17}H_{12}N_4O_2$ 304.307
Mp 273-276°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 894C (*ir*)

Kuhn, R. *et al., Ber.*, 1934, **67**, 1459; 1935, **68**, 1282 (*Isoalloxazine derivs*)
Tishler, M. *et al., J.A.C.S.*, 1945, **67**, 2165 (*synth*)
Lambooy, J.P. *et al., Heterocycl. Compd.*, (ed. Elderfield, R.C.) Wiley, New York, 1967, **9**, 118 (*rev*)
Szymusiak, H. *et al., J.C.S. Perkin 2*, 1990, 229 (*struct, props*)
Villemin, D. *et al., Synth. Commun.*, 1995, **25**, 2315 (*synth*)
Kaupp, G. *et al., Eur. J. Org. Chem.*, 2002, 1368-1373 (*synth, ir, pmr, cmr*)
Chattopadhyay, P. *et al., Synth. Commun.*, 2006, **36**, 1857-1861 (*10-benzyl*)

Almazole A A-633



$C_{21}H_{21}N_3O_3$ 363.415

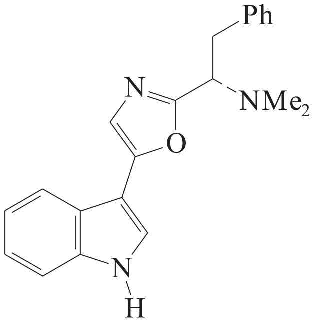
(S)-form [157382-33-7]
Alkaloid from the red alga *Haraldiophyllum* sp. Semisolid. $[\alpha]_D^{20}$ +103 (c, 0.155 in MeOH). λ_{max} 204 (ϵ 36700); 237 (ϵ 26400); 278 (ϵ 18200); 320 (ϵ 6000) (MeOH) (Derep).

Deformyl: ***Almazole B***
[157382-34-8]
$C_{20}H_{21}N_3O_2$ 335.405
Alkaloid from *Haraldiophyllum* sp. Yellow semisolid. $[\alpha]_D^{20}$ +92 (c, 0.05 in MeOH). λ_{max} 203 (ϵ 40300); 234 (ϵ 22600); 260 (ϵ 16500); 396 (ϵ 6300) (MeOH) (Derep).

N'Diaye, I. *et al., Tet. Lett.*, 1994, **35**, 4827-4830 (*isol, uv, cd, pmr, cmr, ms*)
Khalafy, J. *et al., Aust. J. Chem.*, 1999, **52**, 31-36 (*synth*)

Almazole C A-634

[161068-69-5]

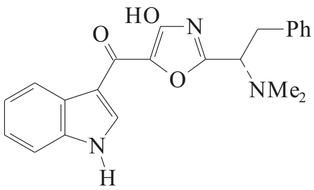


$C_{21}H_{21}N_3O$ 331.416
Alkaloid from the red alga *Haraldiophyllum* sp. CNS active. $[\alpha]_D^{20}$ +168 (c, 1.08 in MeOH). λ_{max} 222 (ϵ 26000); 271 (ϵ 15100); 282 (ϵ 14500); 300 (ϵ 12900) (MeOH) (Berdy).

Guella, G. *et al., Helv. Chim. Acta*, 1994, **77**, 1999-2006 (*isol, synth, cd, uv, pmr, cmr, ms*)

Almazole D A-635

[176739-66-5]



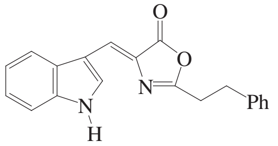
$C_{22}H_{21}N_3O_3$ 375.426
Alkaloid from the red alga *Haraldiophyllum* sp. Shows antifungal activity. Powder. $[\alpha]_D^{20}$ +20 (c, 0.07 in MeOH).

Me ether:
Powder. $[\alpha]_D^{20}$ +70 (c, 0.1 in MeOH).

N'Diaye, I. *et al., Tet. Lett.*, 1996, **37**, 3049-3050 (*isol, uv, pmr, cmr, ms*)

Almazolone A-636

[878143-16-9]
[878143-15-8 (*Z*-form), 878143-13-6 (*E*–form)]



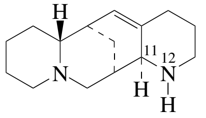
(*Z*)-*form*

$C_{20}H_{16}N_2O_2$ 316.359
Isol. from the red alga *Haraldiophyllum* sp. Yellow powder. Mp 245-247°. Isol. as an 80:20 mixt. of (*Z*/*E*)-isomers to which data refers.

Guella, G. *et al., Tetrahedron*, 2006, **62**, 1165-1170 (*isol, synth, pmr, cmr, ms*)

Aloperine A-637

16,17-Didehydro-9-de-2-piperidinylormosanine, 9CI. Allopterin
[56293-29-9]



Absolute Configuration

$C_{15}H_{24}N_2$ 232.368
Alkaloid from seeds and green parts of *Sophora alopecuroides* (Fabaceae). Large prisms (petrol). Mp 73-75° (70-71°). $[\alpha]_D^{20}$ +82.1 (c, 0.85 in EtOH). Incorr. stereochem. assigned in CA (1997).

▶RM2979500

Hydrochloride: Mp 208°.

Hydrochloride (1:2): Mp 265°.

N-*Benzoyl:*
Cryst. (Et_2O). Mp 161-162°.

N-*Me:* **N-*Methylaloperine***
[63128-33-6]
$C_{16}H_{26}N_2$ 246.395
Alkaloid from *Sophora alopecuroides* (Fabaceae). Mp 94-95°. $[\alpha]_D$ +140 (EtOH).

N-*(2-Propenyl):* **N-*Allylaloperine***
[56595-96-1]
$C_{18}H_{28}N_2$ 272.433
Alkaloid from *Sophora alopecuroides* (Fabaceae). Oil. Mp 235-237° (as hydrobromide)(synthetic).

11,12-Didehydro: ***11,12-Didehydroaloperine***
[142808-31-9]
$C_{15}H_{22}N_2$ 230.352
Alkaloid from leaves and stalks of *Sophora alopecuroides* (Fabaceae).

5,6,11,12,13,14,15,16-Octadehydro: ***5,6,11,12,13,14,15,16-Octadehydroaloperine***
$C_{15}H_{16}N_2$ 224.305
Alkaloid from *Sophora alopecuroides.* Oil. Unpublished data (1999).

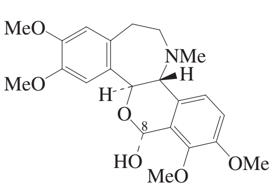
Stereoisomer(1)(?): **Sophora alopecuroides *Alkaloid A₁***. Sophora alopecuroides *Base A₁*
$C_{15}H_{24}N_2$ 232.368
Alkaloid from *Sophora alopecuroides* (Fabaceae). Cryst. (Me_2CO). Mp 92°. $[\alpha]_D$ +195.5 (MeOH).

Stereoisomer(2)(?): **Sophora alopecuroides *Alkaloid A₂***. Sophora alopecuroides *Base A₂*
$C_{15}H_{24}N_2$ 232.368
Alkaloid from *Sophora alopecuroides* (Fabaceae). Cryst. (petrol). Mp 206-208°. $[\alpha]_D$ +25.5 ($CHCl_3$). Possibly the 11-epimer of Aloperine, since it gave the same salts but a different *N*-Me deriv.

Orechoff, A. *et al., Ber.*, 1935, **68**, 431 (*isol*)
Aslanov, Kh.A. *et al., CA*, 1965, **63**, 2050h (*stereoisomers*)
Tolkachev, O.N. *et al., Khim. Prir. Soedin.*, 1975, **11**, 30; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 29 (*ms, pmr, struct*)
Kuchkarov, S. *et al., Khim. Prir. Soedin.*, 1979, **15**, 413; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 364 (*isol*)
Wang, Z. *et al., Zhiwu Xuebao (Acta Bot. Sin.)*, 1991, **33**, 727; *CA*, **117**, 86697b (*11,12-Didehydroaloperine*)
Brosius, A.D. *et al., Acta Cryst. C*, 1997, **53**, 1510-1512 (*cryst struct, abs config*)
Brosius, A.D. *et al., J.O.C.*, 1997, **62**, 440 (*abs config, synth*)
Brosius, A.D. *et al., J.A.C.S.*, 1999, **121**, 700-709 (*synth*)
Passarella, D. *et al., Org. Lett.*, 2002, **4**, 2925-2928 (*synth*)

Alpinigenine A-638

2,3,10,11-Tetramethoxy-16-methylrheadan-8-ol, 9CI. Alkaloid E†



(+)-*form*

$C_{22}H_{27}NO_6$ 401.458
Biogenetic numbering shown. Other systems also used.

(+)-*form* [14028-91-2]
Alkaloid from *Papaver alpinum* various ssp., *Papaver bracteatum, Papaver fugax* (= *Papaver aucasicum*), *Papaver orientale*

and *Papaver pseudo-orientale* (Papaveraceae). Prismatic cryst. (C_6H_6/MeOH or EtOAc). Mp 193-195° (186.5-187.5°). $[\alpha]_D^{22}$ +286 (c, 0.63 in MeOH). $[\alpha]_D^{22}$ +306 (c, 1.08 in MeOH).

Hydrochloride: Mp 161-163° dec. $[\alpha]_D^{18}$ +210 (c, 0.796 in MeOH).

Me ether: ***Epialpinine***. O-*Methylalpinigenine*
[15210-99-8]
$C_{23}H_{29}NO_6$ 415.485
Alkaloid from *Papaver alpinum*, various ssp. (Papaveraceae). Cryst. (MeOH aq.). Mp 105-106° Mp 122-123°. $[\alpha]_D^{18}$ +302 (c, 0.511 in MeOH).

Et ether: **O-*Ethylalpinigenine***
$C_{24}H_{31}NO_6$ 429.512
Isol. from *Papaver fugax* (Papaveraceae). Prob. an artifact.

8-Epimer, Me ether: ***Alpinine***†. N-*Methylpapaverrubine G*
[14028-90-1]
$C_{23}H_{29}NO_6$ 415.485
Alkaloid from *Papaver alpinum*, various ssp., *Papaver bracteatum* and *Papaver pseudo-orientale* (Papaveraceae). Noncryst. $[\alpha]_D^{22}$ +288 (c, 0.82 in $CHCl_3$).

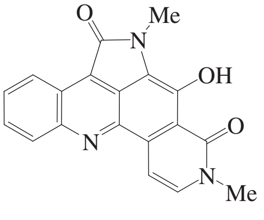
8-Epimer, Me ether, N-*de-Me:* ***Papaverrubine G***. N-*Demethylalpinine*
[17597-20-5]
$C_{22}H_{27}NO_6$ 401.458
Alkaloid from *Papaver alpinum*, various ssp., and *Papaver anomalum* (*Papaver nudicaule* ssp. *amurense*) (Papaveraceae). $[\alpha]_D$ +397 (c, 0.12 in MeOH). Indefinite Mp.

(±)-*form* [40170-39-6]
Synthetic. Needles (EtOAc). Mp 172-173° (168-169°).

Maturová, M. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 419 (*ir, pmr, ms, struct*)
Pfeifer, S. *et al., Pharmazie*, 1967, **22**, 343; 1968, **23**, 585; 1972, **27**, 48 (*Papaverrubine G*)
Dolejš, L. *et al., Tetrahedron*, 1967, **23**, 2997 (*ms*)
Irie, H. *et al., J.C.S. Perkin 1*, 1972, 2986 (*synth*)
Rönsch, H. *et al., Helv. Chim. Acta*, 1977, **60**, 2402 (*Epialpinine*)
Meshulam, H. *et al., Phytochemistry*, 1980, **19**, 2633 (*isol*)
Lavie, D. *et al., J.C.S. Perkin 1*, 1981, 1019 (*isol, cmr, cryst struct, abs config*)
Prabhaker, S. *et al., J.C.S. Perkin 1*, 1981, 1273 (*synth*)
Phillipson, J.D. *et al., Planta Med.*, 1981, **43**, 105; 261 (*O-Ethylalpinigenine*)
Hanaoka, M. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2273 (*synth*)

Alpkinidine A-639

[486992-29-4]



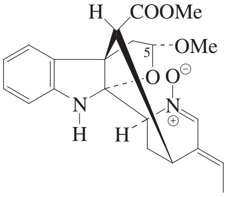
$C_{19}H_{13}N_3O_3$ 331.33

Alkaloid from *Xestospongia* cf. *carbonaria*. Purple solid.

Thale, Z. *et al., J.O.C.*, 2002, **67**, 9384-9391 (*isol, pmr, cmr, cryst struct*)

Alschomine A-640

[123045-72-7]



Absolute Configuration

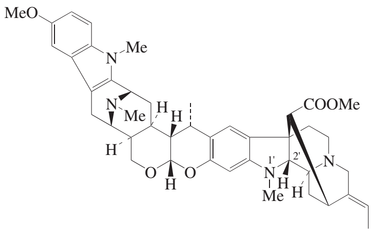
$C_{21}H_{24}N_2O_5$ 384.431
Alkaloid from the leaves of *Alstonia scholaris* (Apocynaceae). Prisms (MeOH). Mp 233-240° dec. $[\alpha]_D^{27}$ +116.1 (c, 0.25 in MeOH).

5-Epimer: ***Isoalschomine***
[123062-73-7]
$C_{21}H_{24}N_2O_5$ 384.431
Alkaloid from leaves of *Alstonia scholaris* (Apocynaceae). Prisms (MeOH). Mp 220-230° dec. $[\alpha]_D^{27}$ +112.3 (c, 0.14 in MeOH).

Abe, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 887 (*isol, uv, pmr, cmr, cryst struct*)

Alstocraline A-641

[120416-01-5]



Absolute Configuration

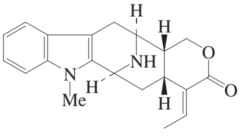
$C_{43}H_{52}N_4O_5$ 704.908
Alkaloid from the leaves of *Alstonia angustifolia* (Apocynaceae). $[\alpha]_D$ +3 (c, 0.7 in MeOH). λ_{max} 227 (log ϵ 4.02); 282 (log ϵ 4.45); 295 (sh) (log ϵ 4.44) (MeOH).

*1′-*N*-De-Me, 1′,2′-didehydro:* ***Foliacraline***
[120374-18-7]
$C_{42}H_{48}N_4O_5$ 688.865
Alkaloid from the leaves of *Alstonia angustifolia* (Apocynaceae). $[\alpha]_D$ +55 (c, 0.3 in $CHCl_3$). λ_{max} 220 ; 228 ; 289 ; 302 (sh) (MeOH).

Ghedira, K. *et al., Phytochemistry*, 1988, **27**, 3955-3962 (*isol, uv, ir, pmr, cmr, ms, struct*)

Alstolactone A-642

[701950-29-0]



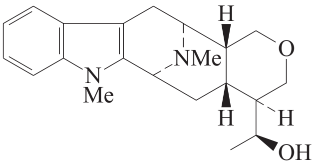
Absolute Configuration

$C_{20}H_{22}N_2O_2$ 322.406
Alkaloid from the leaves of *Alstonia angustifolia* var. *latifolia*. Light yellow oil. $[\alpha]_D$ -10 (c, 0.05 in $CHCl_3$). λ_{max} 216 (log ϵ 4.23); 228 (log ϵ 4.3); 284 (log ϵ 3.76); 293 (log ϵ 3.71) (EtOH).

Kam, T.-S. *et al., Phytochemistry*, 2004, **65**, 603-608 (*isol, pmr, cmr*)

Alstomacroine A-643

[160866-97-7]

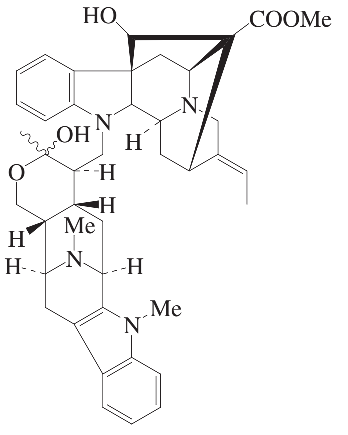


$C_{21}H_{28}N_2O_2$ 340.464
Alkaloid from the leaves of *Alstonia macrophylla*. $[\alpha]_D$ +2.6 (c. 0.02 in $CHCl_3$). λ_{max} 230 (log ϵ 4.6); 285 (log ϵ 4.5) (MeOH).

Atta-ur-Rahman, *et al., Nat. Prod. Lett.*, 1994, **5**, 201-209 (*isol, pmr, cmr, ms*)

Alstomacroline A-644

[199800-14-1]

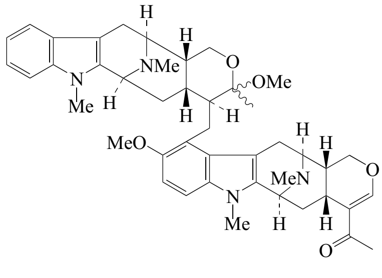


$C_{42}H_{50}N_4O_5$ 690.881
Alkaloid from the root bark of *Alstonia macrophylla*. Amorph. powder. $[\alpha]_D^{20}$ +54.6 (c, 0.4 in $CHCl_3$). λ_{max} 232 (log ϵ 4.44); 251 (log ϵ 3.88); 293 (log ϵ 3.78) (MeOH).

Keawpradub, N. *et al., Phytochemistry*, 1997, **46**, 757-762 (*isol, uv, ir, pmr, cmr, ms*)

Alstomacrophylline A-645

[199800-12-9]

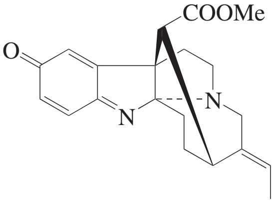


$C_{44}H_{54}N_4O_5$ 718.934
Alkaloid from the root bark of *Alstonia macrophylla* (Apocynaceae). Amorph. powder. $[\alpha]_D^{20}$ +42.8 (c, 0.09 in MeOH). λ_{max} 232 (log ϵ 4.27); 260 (log ϵ 3.67); 292 (log ϵ 3.51) (MeOH).

Keawpradub, N. *et al., Phytochemistry*, 1997, **46**, 757-762 (*isol, uv, ir, pmr, cmr, ms*)

Alstomaline A-646

[685508-21-8]

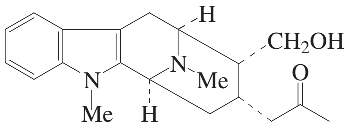


$C_{20}H_{22}N_2O_3$ 338.405
Represents a new structural subtype related to the akuammiline alkaloids, which has however been found previously in a small number of dimers, e.g. Flexicorine, F-88. Alkaloid from the leaves of *Alstonia macrophylla*. Yellowish oil. $[\alpha]_D$ -244 (c, 0.04 in $CHCl_3$). λ_{max} 202 (log ϵ 3.77); 273 (log ϵ 3.85); 317 (log ϵ 3.12) (EtOH).

Kam, T.-S. *et al., J. Nat. Prod.*, 2004, **67**, 547-552 (*isol, pmr, cmr*)

Alstomicine A-647

[5594-43-4]

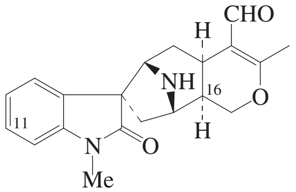


$C_{20}H_{26}N_2O_2$ 326.438
Alkaloid from the leaves of *Alstonia macrophylla*. Light yellowish oil. $[\alpha]_D$ +74 (c, 0.14 in $CHCl_3$). λ_{max} 230 (log ϵ 3.8); 289 (log ϵ 3.11) (EtOH).

Kam, T.-S. *et al., J. Nat. Prod.*, 2004, **67**, 547-552 (*isol, pmr, cmr, ms*)

Alstonal A-648

20-Deacetyl-20-formyl-17-methylalstonisine, 9CI
[172924-28-6]



$C_{20}H_{22}N_2O_3$ 338.405
Alkaloid from bark of *Alstonia macrophylla*. Needles (petrol/Me_2CO). Mp 198-199°. $[\alpha]_D$ +167 (c, 0.062 in $CHCl_3$).

N-De-Me: ***N-Demethylalstonal***
[301323-29-5]
$C_{19}H_{20}N_2O_3$ 324.379
Alkaloid from *Alstonia macrophylla*. Not obt. pure.

16-Hydroxy: ***16-Hydroxyalstonal***
[683239-99-8]
$C_{20}H_{22}N_2O_4$ 354.405
Alkaloid from the leaves of *Alstonia macrophylla*. Amorph. powder. $[\alpha]_D$ +153 (c, 0.26 in $CHCl_3$). λ_{max} 207 (log ϵ 4.61); 263 (log ϵ 4.35) (EtOH).

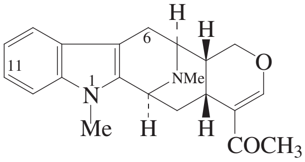
11-Methoxy: **N^b*-Demethylalstophyllal oxindole***. *11-Methoxyalstonal*
[172927-64-9]
$C_{21}H_{24}N_2O_4$ 368.432
From bark of *Alstonia macrophylla*. Needles (petrol/Me_2CO). Mp 190-191°. $[\alpha]_D$ +174 (c, 0.063 in $CHCl_3$).

11-Methoxy, 16-hydroxy: ***16-Hydroxy-11-methoxyalstonal***
[683240-00-8]
$C_{21}H_{24}N_2O_5$ 384.431
Alkaloid from the leaves of *Alstonia macrophylla*. Amorph. powder. $[\alpha]_D$ +203 (c, 0.11 in $CHCl_3$). λ_{max} 220 (log ϵ 4.54); 267 (log ϵ 4.2) (EtOH).

Wong, W.-H. *et al., Phytochemistry*, 1996, **41**, 313 (*isol, pmr, cmr, ms, struct*)
Kam, T.-S. *et al., Tetrahedron*, 2000, **56**, 6143-6150 (*N-Demethylalstonal*)
Kam, T.-S. *et al., J. Nat. Prod.*, 2004, **67**, 547-552 (*16-Hydroxyalstonal, 16-Hydroxy-11-methoxyalstonal*)

Alstonerine A-649

Alstophyllan-19-one, 9CI. Alkaloid D†
[25921-22-6]



$C_{21}H_{24}N_2O_2$ 336.433
Alkaloid from bark of *Alstonia muelleriana* (Apocynaceae). Cryst. (Et_2O). Mp 172-173°. $[\alpha]_D^{25}$ -195 (c, 0.6 in EtOH).

N^4*-De-Me:* **N^4*-Demethylalstonerine***
[701304-79-2]
$C_{20}H_{22}N_2O_2$ 322.406
Alkaloid from the leaves of *Alstonia angustifolia* var. *latifolia*.

11-Methoxy: ***Alstophylline***
[3382-41-0]
$C_{22}H_{26}N_2O_3$ 366.459
Alkaloid from *Alstonia macrophylla* and *Alstonia glabriflora* (Apocynaceae). Cryst. (CH_2Cl_2/hexane). Mp 155-158°. $[\alpha]_D^{26}$ -151 (c, 0.326 in MeOH).

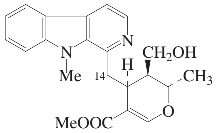
11-Methoxy, N^1*-de-Me:* **N^1*-Demethylalstophylline***
$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from the bark of *Alstonia macrophylla*.

11-Methoxy, 6-oxo: ***6-Oxoalstophylline***
[683240-01-9]
$C_{22}H_{24}N_2O_4$ 380.443
Alkaloid from the leaves of *Alstonia macrophylla*.

Kishi, T. *et al., Helv. Chim. Acta*, 1965, **48**, 1349; 1966, **49**, 946 (*Alstonerine, Alstophylline, isol, uv, ir, pmr, struct, synth*)
Cook, J.M. *et al., Chem. Comm.*, 1969, 1306 (*uv, ir, pmr, ms, struct*)
Hart, N.K. *et al., Aust. J. Chem.*, 1972, **25**, 2739 (*Alstophylline, isol*)
Elderfield, R.C. *et al., Phytochemistry*, 1972, **11**, 339 (*isol, ir, uv*)
Garnick, R.L. *et al., J.A.C.S.*, 1978, **100**, 4213 (*synth, ms*)
Zhang, L.H. *et al., J.A.C.S.*, 1990, **112**, 4088 (*synth*)
Takayama, H. *et al., Tetrahedron*, 1991, **47**, 1383 (*synth*)
Bi, Y. *et al., J.A.C.S.*, 1994, **116**, 9027 (*synth*)
Yu, P. *et al., J.O.C.*, 2000, **65**, 3173-3191 (*synth*)
Kam, T.-S. *et al., J. Nat. Prod.*, 2004, **67**, 547-552 (*6-Oxoalstophylline*)
Kam, T.-S. *et al., Phytochemistry*, 2004, **65**, 603-608 (*N^4-Demethylalstonerine*)
Kam, T.-S. *et al., Tetrahedron*, 2004, **60**, 3957-3966 (*N^1-Demethylalstophylline*)
Tran, Y.S. *et al., Org. Lett.*, 2005, **7**, 4289-4291 (*synth*)
Liao, X. *et al., J.O.C.*, 2006, **71**, 8884-8890 (*synth*)
Miller, K.A. *et al., Org. Lett.*, 2007, **9**, 1113-1116 (*synth*)

Alstonidine A-650

[25394-75-6]



Relative Configuration

$C_{22}H_{24}N_2O_4$ 380.443
Alkaloid from *Alstonia constricta* (Apocynaceae). Mp 188-190°. $[\alpha]_D$ -99 (c, 1.0 in $CHCl_3$).

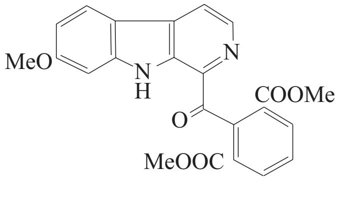
Ac:
Needles + $3H_2O$ (Me_2CO aq.). Mp 92-96°.

14-Oxo: ***14-Ketoalstonidine***
$C_{22}H_{22}N_2O_5$ 394.426
Alkaloid from stem bark of *Alstonia constricta* (Apocynaceae). Noncryst. Labile.

Boaz, H. *et al., J. Am. Pharm. Assoc.*, 1957, **46**, 510 (*isol, uv, ir, struct*)
Crow, W.D. *et al., Aust. J. Chem.*, 1970, **23**, 2489 (*isol, pmr, ms, config*)
Allam, K. *et al., J. Nat. Prod.*, 1987, **50**, 623 (*14-Ketoalstonidine*)

Alstonilidine A-651

[31185-76-9]



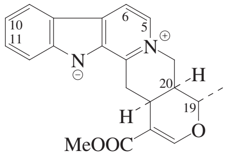
$C_{23}H_{18}N_2O_6$ 418.405
A secoyohimbane. Alkaloid from the

root bark of *Alstonia constricta* (Apocynaceae). Needles (EtOH). Mp 244-245°.

Crow, W.D. *et al., Aust. J. Chem.*, 1970, **23**, 2489 (*isol, uv, ir, pmr, ms, struct*)

Alstonine **A-652**

[47485-83-6]



Absolute Configuration

$C_{21}H_{20}N_2O_3$ 348.401

The early history of alkaloids called Alstonine is confused. Alkaloid from *Alstonia constricta*, *Rauwolfia obscura*, *Rauwolfia volkensii*, *Rauwolfia nitida*, *Rauwolfia serpentina*, *Catharanthus roseus*, *Strychnos camptoneura* and *Strychnos gossweileri* (Apocynaceae, Loganiaceae). Shows neoplasm-inhibiting props. Mp 205-210° dec. λ_{max} 252 ; 289 ; 309 ; 336 ; 369 (MeOH) (Berdy).

Hydrochloride: Mp 278-279° dec.

Perchlorate: Mp 239-240°. $[\alpha]_D^{20}$ +154 (Me_2CO).

10,11-Dimethoxy: ***Bleekerine***. *10,11-Dimethoxyalstonine*
[41758-43-4]
$C_{23}H_{24}N_2O_5$ 408.453
Alkaloid from the stem bark of *Bleekeria vitiensis* (preferred genus name *Ochrosia*) (Apocynaceae). Pale yellow prisms (EtOH). Mp 276-277°. $[\alpha]_{Hg}^{22.5}$ +612 (MeOH).

10,11-Dimethoxy, 5,6-dihydro: ***Ochropposine***
[38146-72-4]
$C_{23}H_{26}N_2O_5$ 410.469
Alkaloid from the bark of *Ochrosia oppositifolia* and *Ochrosia moorei* (Apocynaceae). Mp 312-314° dec. (as perchlorate). λ_{max} 222 (log ϵ 4.44); 401 (log ϵ 4.43) (no solvent reported) (perchlorate).

19-Epimer: ***19-Epialstonine***
$C_{21}H_{20}N_2O_3$ 348.401
Alkaloid from the roots of *Amphicome emodi* (preferred genus name *Incarvillea*). Cryst. Mp 245° dec.

20-Epimer: ***Serpentine***
[18786-24-8]
$C_{21}H_{20}N_2O_3$ 348.401
Alkaloid from *Rauwolfia serpentina* and many other *Rauwolfia* spp., *Strychnos camptoneura*, *Catharanthus roseus*, *Catharanthus ovalis* and *Vinca major* (Apocynaceae). Shows antitumour activity. Mp 156-157° dec. (170°). $[\alpha]_D$ +292 (MeOH). λ_{max} 251 (log ϵ 4.5); 307 (log ϵ 4.31); 368 (log ϵ 3.55) (MeOH).

20-Epimer, hydrochloride: Mp 246-248°. $[\alpha]_D^{25}$ +178 (H_2O).

19,20-Diepimer: ***19-Episerpentine***
[64753-57-7]
$C_{21}H_{20}N_2O_3$ 348.401
Alkaloid from the roots of *Rauwolfia cumminsii* (Apocynaceae). Yellow cryst. powder. Mp 240° dec.

19,20-Diepimer, 11-methoxy: ***Serpenticine***
[81149-04-4]
$C_{22}H_{22}N_2O_4$ 378.427
Alkaloid from *Rauwolfia vomitoria* (Apocynaceae). Yellow plates + $5H_2O$ ($MeOH/C_6H_6$). Mp 275-276°. λ_{max} 265 (log ϵ 4.4); 310 (log ϵ 4.2); 365 (log ϵ 3.6) (no solvent reported).

19,20-Diepimer, 11-methoxy, hydrochloride: Mp 289-290°.

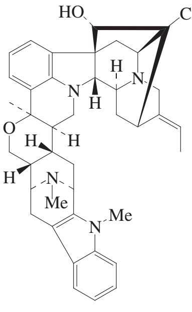
19,20-Diepimer, 11-methoxy, picrate: Mp 196-198°.

[642-18-2]

Sharp, T.M. *et al., J.C.S.*, 1934, 287-291 (*isol*)
Raymond-Hamet, *et al., C. R. Hebd. Seances Acad. Sci.*, 1948, **227**, 344-345 (*uv*)
Elderfield, R.C. *et al., J.O.C.*, 1951, **16**, 506-523 (*struct*)
Schlittler, E. *et al., Helv. Chim. Acta*, 1952, **35**, 271-276; 1954, **37**, 1912-1920 (*isol, Serpentine, uv, ir, struct*)
Bader, F.E. *et al., Helv. Chim. Acta*, 1953, **36**, 215-226 (*struct*)
Wenkert, E. *et al., J.A.C.S.*, 1957, **79**, 1519-1520; 1958, **80**, 1613-1619 (*config, synth*)
Fritz, H. *et al., Annalen*, 1962, **655**, 148-167 (*Serpentine, config, ir, uv*)
Saxton, J.E. *et al., Alkaloids (Academic Press)*, 1965, **8**, 159-202 (*bibl*)
Battersby, A.R. *et al., Chem. Comm.*, 1966, 888-890 (*biosynth*)
Peube-Locou, N. *et al., Phytochemistry*, 1972, **11**, 2109-2111 (*Ochropposine*)
Sainsbury, M. *et al., Phytochemistry*, 1972, **11**, 2337-2339 (*Bleekerine*)
Timmins, P. *et al., Phytochemistry*, 1976, **15**, 733-735 (*isol*)
Iwu, M.M. *et al., Planta Med.*, 1977, **32**, 158-161 (*19-Episerpentine*)
Malik, A. *et al., Heterocycles*, 1981, **16**, 1727-1733 (*Serpenticine*)
Ahond, A. *et al., J. Nat. Prod.*, 1981, **44**, 193-199 (*Ochropposine, isol*)
Dinda, B. *et al., Indian J. Chem., Sect. B*, 2002, **41**, 2698-2700 (*19-Epialstonine*)
Wachsmuth, O. *et al., Phytochemistry*, 2002, **61**, 705-709 (*Serpentine, isol, pmr, cmr, ms*)

Alstonisidine **A-653**

[36474-13-2]



Absolute Configuration

$C_{42}H_{48}N_4O_4$ 672.866

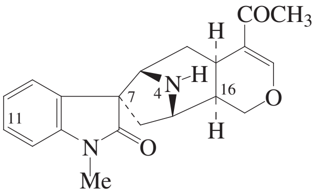
Alkaloid from the bark of *Alstonia muelleriana* (Apocynaceae). Rods (MeOH). Mp 325° dec. $[\alpha]_D$ -234 (c, 1.0 in EtOH). $[\alpha]_D$ -133 (c, 0.208 in $CHCl_3$) (natural). $[\alpha]_D$ -144 (c, 0.335 in $CHCl_3$) (synthetic).

Hydrochloride (1:2):
Cryst. (MeOH). Mp 268° (dec. *in vacuo*). $[\alpha]_D^{25}$ +137 (c, 0.6 in H_2O).

Cook, J.M. *et al., J.O.C.*, 1971, **36**, 582 (*uv, ir, pmr, ms*)
Elderfield, R.C. *et al., Phytochemistry*, 1972, **11**, 339 (*isol, uv, ir*)
Burke, D.E. *et al., J.A.C.S.*, 1973, **95**, 546 (*synth, struct*)
Hoard, L.D. *et al., Diss. Abstr. Int., B*, 1977, **38**, 2690 (*cryst struct*)

Alstonisine, 9CI **A-654**

Alkaloid C†
[35804-91-2]



$C_{20}H_{22}N_2O_3$ 338.405

Alkaloid from the bark of *Alstonia muelleriana* and *Alstonia macrophylla* (Apocynaceae). Cryst. (MeOH aq.). Mp 168-169°. $[\alpha]_D^{25}$ +200 (c, 1.0 in EtOH).

Hydrochloride: Mp 250-260° dec. $[\alpha]_D^{25}$ +155 (c, 1.0 in H_2O).

N^4-*Formyl:* N^4-*Formylalstonisine*. ***Alstofoline***
[301521-97-1]
$C_{21}H_{22}N_2O_4$ 366.416
Alkaloid from *Alstonia macrophylla*. $[\alpha]_D$ +39 (c, 0.21 in $CHCl_3$). λ_{max} 214 (log ϵ 4.02); 246 (log ϵ 4.01); 254 (log ϵ 4.05); 290 (log ϵ 3.13) (EtOH).

N-De-Me: ***N-Demethylalstonisine***
[301323-28-4]
$C_{19}H_{20}N_2O_3$ 324.379
Alkaloid from *Alstonia macropylla*.

16-Hydroxy: ***16-Hydroxyalstonisine***
[683239-98-7]
$C_{20}H_{22}N_2O_4$ 354.405
Alkaloid from the leaves of *Alstonia macrophylla*. Amorph. powder. $[\alpha]_D$ +170 (c, 0.15 in $CHCl_3$). λ_{max} 209 (log ϵ 4.17); 256 (log ϵ 3.95) (EtOH).

11-Methoxy: ***N^b-Demethylalstophylline oxindole***
[108195-73-9]
$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from leaves and bark of *Alstonia macrophylla*. Prisms (petrol/Me_2CO). Mp 205-206°. $[\alpha]_D$ +126 (c, 0.068 in $CHCl_3$).

11-Methoxy, 16-hydroxy: ***16-Hydroxy-N^b-demethylalstophylline oxindole***. *14-Hydroxy-11-methoxyalstonisine, 9CI*
[114466-39-6]
$C_{21}H_{24}N_2O_5$ 384.431
Alkaloid from leaves of *Alstonia macrophylla*. Mp 215°. $[\alpha]_D$ +104.47 (c, 0.067 in $CHCl_3$).

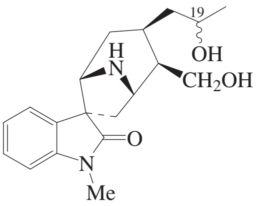
7-Epimer: ***Isoalstonisine***
[301521-98-2]
$C_{20}H_{22}N_2O_3$ 338.405
Alkaloid from *Alstonia macrophylla*. $[\alpha]_D$ +207 (c, 0.07 in $CHCl_3$). λ_{max} 210 (log ϵ 3.93); 255 (log ϵ 3.8) (EtOH).

Nordman, C.E. *et al., J.A.C.S.*, 1963, **85**, 353 (*cryst struct*)
Elderfield, R.C. *et al., Phytochemistry*, 1972, **11**, 339 (*isol, uv, ir*)

Atta-ur-Rahman, *et al., Phytochemistry*, 1987, **26**, 865 (*N^b-Demethylalstophylline oxindole*)
Atta-ur-Rahman, *et al., Heterocycles*, 1988, **27**, 725 (*16-Hydroxy-N^b-demethylalstophylline oxindole*)
Wong, W.-H. *et al., Phytochemistry*, 1996, **41**, 313 (*N^b-Demethylalstophylline oxindole*)
Kam, T.-S. *et al., Tetrahedron*, 2000, **56**, 6143-6150 (*Isoalstonisine, N-Demethylalstonisine, Alstofoline*)
Wearing, X.Z. *et al., Org. Lett.*, 2002, **4**, 4237-4240 (*synth*)
Kam, T.-S. *et al., J. Nat. Prod.*, 2004, **67**, 547-552 (*16-Hydroxyalstonisine*)

Alstonoxine B A-655

[301521-96-0]



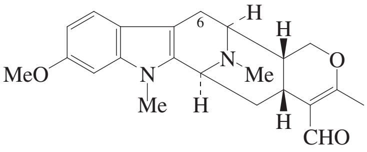
$C_{19}H_{26}N_2O_3$ 330.426
Alkaloid from *Alstonia macrophylla*. $[\alpha]_D$ -12 (c, 0.41 in $CHCl_3$). λ_{max} 213 (log ϵ 4.15); 255 (log ϵ 3.65) (EtOH).

19-Ketone: ***Alstonoxine A***
[301521-95-9]
$C_{19}H_{24}N_2O_3$ 328.41
Alkaloid from *Alstonia macrophylla*. $[\alpha]_D$ -34 (c, 0.19 in $CHCl_3$). λ_{max} 216 (log ϵ 3.89); 255 (log ϵ 3.7); 285 (log ϵ 3.18) (EtOH).

Kam, T.-S. *et al., Tetrahedron*, 2000, **56**, 6143-6150

Alstophyllal A-656

[685508-23-0]

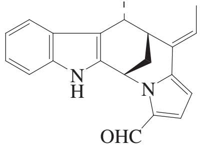


$C_{22}H_{26}N_2O_3$ 366.459
Alkaloid from the leaves of *Alstonia macrophylla*.

6-Oxo: ***6-Oxoalstophyllal***
[683240-02-0]
$C_{22}H_{24}N_2O_4$ 380.443
Alkaloid from the leaves of *Alstonia macrophylla*.

Kam, T.-S. *et al., J. Nat. Prod.*, 2004, **67**, 547-552 (*isol, pmr, cmr*)

Alstoscholarine A-657



Absolute Configuration

(*E*)-form

$C_{22}H_{20}N_2O_3$ 360.412

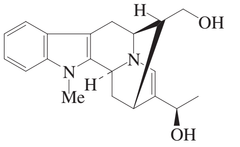
(E)-form [937245-47-1]
Alkaloid from the leaves of *Alstonia scholaris*. Green prisms. Mp 168-170°. $[\alpha]_D^{20}$ -53 (c, 0.065 in $CHCl_3$). λ_{max} 223 ; 291 ; 300 ($CHCl_3$).

(Z)-form [937245-48-2]
Alkaloid from the leaves of *Alstonia scholaris*. Powder. $[\alpha]_D^{25}$ -140 (c, 0.05 in $CHCl_3$). λ_{max} 220 ; 286 ; 293 ($CHCl_3$).

Cai, X.-H. *et al., Org. Lett.*, 2007, **9**, 1817-1820 (*isol, pmr, cmr, cryst struct*)

Alstoumerine A-658

[135824-73-6]



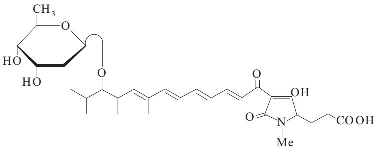
Absolute Configuration

$C_{20}H_{24}N_2O_2$ 324.422
Alkaloid from *Alstonia macrophylla* (Apocynaceae). Pale yellow cryst. Mp 170°. $[\alpha]_D$ -5.5 (c, 0.0034 in $CHCl_3$).

Atta-ur-Rahman, *et al., J. Nat. Prod.*, 1991, **54**, 750-754 (*isol, uv, ir, pmr, cmr, ms, struct*)

Altamycin A A-659

[60202-22-4]

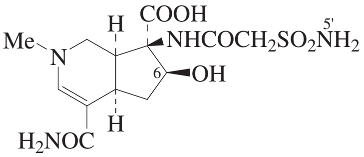


$C_{30}H_{43}NO_9$ 561.671
Polyene-type antibiotic. Sol. MeOH, EtOH, Me_2CO, DMF, bases, AcOH, Py, butanol; poorly sol. dioxan, MeCN, $CHCl_3$, acids, H_2O, hexane. Mp 140-142°. $[\alpha]_D$ -72 (c, 0.5 in EtOH). No biol. source referred to in abstract. λ_{max} 262 (E1%/1cm 105); 343 (E1%/1cm 400); 355 (E1%/1cm 450); 375 (E1%/1cm 320) (MeOH) (Berdy).

Shenin, Yu.D. *et al., CA*, 1987, **106**, 66971f (*struct*)

Altemicidin A-660

Artemicidine
[125399-82-8]



$C_{13}H_{20}N_4O_7S$ 376.39
Prod. by *Streptomyces sioyaensis*. Possesses acaricidal, miticidal and antitumour activities. Powder. Sol. H_2O; fairly sol. MeOH, EtOH; poorly sol. Me_2CO, hexane. Mp 195-199° dec. $[\alpha]_D^{27}$ -7.6 (c, 1 in H_2O). λ_{max} 305 (ϵ 11300) (0.1*M* HCl) (Derep). λ_{max} 300 (ϵ 20800) (0.1*M* NaOH) (Derep). λ_{max} 300 (ϵ 20300) (pH 6.8 phosphate buffer) (Derep).

▶ LD_{50} (mus, ivn) 0.3 mg/kg. UW8797000

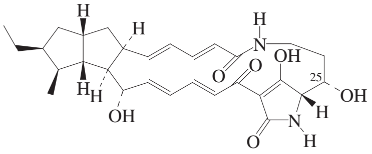
*5′-*N*-(2*S*-Amino-3*S*-methylpentanoyl):* ***Antibiotic SB 203207***. *SB 203207*
$C_{19}H_{31}N_5O_8S$ 489.549
Prod. by *Streptomyces* sp. NCIMB 40513. Isoleucyl tRNA synthetase inhibitor. Powder. λ_{max} 299 (H_2O).

*5′-*N*-(2*S*-Amino-3*S*-methylpentanoyl), 6-*O*-(2*S*-amino-3*S*-phenylbutanoyl):* ***Antibiotic SB 203208***. *SB 203208*
$C_{29}H_{42}N_6O_9S$ 650.752
Prod. by *Streptomyces* sp. NCIMB 40513. Isoleucyl tRNA synthetase inhibitor. Powder. λ_{max} 297 (H_2O).

Takahashi, A. *et al., J. Antibiot.*, 1989, **42**, 1556-1561; 1562-1566 (*isol, struct*)
Takahashi, A. *et al., Tetrahedron*, 1991, **47**, 3621-3632 (*pmr, cmr*)
Kende, A.S. *et al., J.A.C.S.*, 1995, **117**, 10597-10598 (*synth*)
Stefanska, A.L. *et al., J. Antibiot.*, 2000, **53**, 357-363 (*SB 203207/8*)
Houge-Frydrych, C.S.V. *et al., J. Antibiot.*, 2000, **53**, 364-372 (*SB 203207/8*)

Alteramide A A-661

[142131-06-4]



$C_{29}H_{38}N_2O_6$ 510.629
Macrocylic lactam antibiotic. Isol. from an *Alteromonas* sp. associated with the sponge *Halichondria okadai*. Exhibits cytotoxicity against murine leukaemia P388 cells, murine lymphoma L1210 cells and the human epidermoid carcinoma KB cells *in vitro*. Yellow powder. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. Mp 200° (dec.). $[\alpha]_D^{22}$ +36.2 (c, 0.1 in MeOH). λ_{max} 268 (ϵ 30300); 347 (ϵ 11000) (MeOH) (Derep).

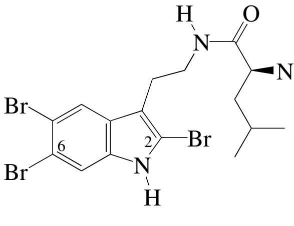
25-Deoxy: ***Alteramide B***
$C_{29}H_{38}N_2O_5$ 494.63
From an *Alteromonas* sp. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. λ_{max} 268 ; 347 (MeOH) (Berdy).

[142131-07-5]

Shigemori, H. *et al., J.O.C.*, 1992, **57**, 4317-4320 (*isol, ir, uv, pmr, cmr, struct*)

Alternatamide B A-662

[191212-58-5]



$C_{17}H_{22}Br_3N_3O$ 524.092

Alkaloid from the marine bryozoan *Amathia alternata*. Moderate antibacterial agent. Amorph. powder.

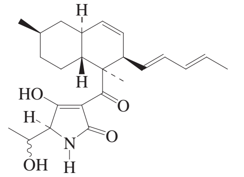
N^1*-Me:* ***Alternatamide A***
[191212-57-4]
$C_{18}H_{24}Br_3N_3O$ 538.119
Alkaloid from *Amathia alternata*. Amorph. powder.

2-Debromo: ***Alternatamide D***
[191212-60-9]
$C_{17}H_{23}Br_2N_3O$ 445.196
Alkaloid from *Amathia alternata*. Amorph. powder.

6-Debromo: ***Alternatamide C***
[191212-59-6]
$C_{17}H_{23}Br_2N_3O$ 445.196
Alkaloid from *Amathia alternata*. Amorph. powder.

Lee, N.-K. *et al., J. Nat. Prod.*, 1997, **60**, 697-699 (*isol, uv, cd, ir, pmr, cmr, ms*)

Altersetin A-663



Absolute Configuration

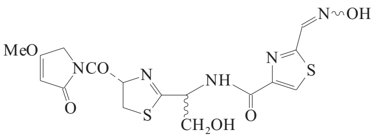
$C_{24}H_{33}NO_4$ 399.529

Tetramic acid antibiotic. Enolised triketone. Related to Equisetin, E-142 and Phomasetin, P-373. Prod. by *Alternaria* spp. P 0506 and P 0535. Active against gram-positive and -negative bacteria and yeasts. Solid. λ_{max} 234 (log ϵ 4.37); 286 (log ϵ 3.84) (MeOH).

Hellwig, V. *et al., J. Antibiot.*, 2002, **55**, 881-892 (*isol, cd, pmr, cmr, ms*)

Althiomycin, 8CI A-664

Matamycin. Antibiotic 116A
[12656-40-5]



$C_{16}H_{17}N_5O_6S_2$ 439.472

Peptide antibiotic. The nat. prod. has the thiazole-ring *S*-config. as illus. but is prob. a mixt. of side-chain diastereoisomers. The oxime config. also appears uncertain although the *Z*-isomer has been prepd. synthetically. Isol. from *Cystobacter fuscus, Myxococcus virescens, Myxococcus xanthus, Streptomyces althioticus, Streptomyces chartreusis* and *Streptomyces matensis.* Active against gram-positive organisms. Also shows anticoccidial and antiherpes activity. Cryst. (CH_2Cl_2/EtOH). Mp 181-184° (dec.). $[\alpha]_D^{25}$ +37.8 (c, 2 in EtOH/CH_2Cl_2). λ_{max} 235 (ϵ 22800); 312 (ϵ 11500) (0.1*N* NaOH) (Derep). λ_{max} 222 (ϵ 36600); 238 (ϵ 28300); 285 (ϵ 8200) (EtOH) (Derep).

▶ LD_{Lo} (mus, ipr) 720 mg/kg.

Yamaguchi, H. *et al., J. Antibiot., Ser. A*, 1957, **10**, 195 (*isol*)
Cram, D.J. *et al., J.A.C.S.*, 1963, **85**, 1430 (*uv, ir, pmr*)
Sakakibara, H. *et al., J. Antibiot.*, 1974, **27**, 897 (*pmr, cmr, cryst struct*)
Pestka, S. *et al., Antibiotics (N.Y.)*, 1975, **3**, 323 (*rev*)
Bycroft, B.W. *et al., Chem. Comm.*, 1975, 121 (*struct, ms, ir, uv, pmr, cmr*)
Kirst, H.A. *et al., J. Antibiot.*, 1975, **28**, 286 (*struct, nmr, ir, uv, ms*)
Kunze, B. *et al., J. Antibiot.*, 1982, **35**, 635 (*isol, bibl*)
Shiba, T. *et al., Tet. Lett.*, 1984, **25**, 2009 (*synth*)
Inami, K. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2185 (*activity, synth, derivs*)
Toogood, P.L. *et al., Bioorg. Med. Chem. Lett.*, 1996, **6**, 1543 (*synth*)

Alvanidine A-665

$C_{20}H_{33}NO_2$ 319.486

Prob. a steroidal alkaloid. Struct. unknown. Alkaloid from *Fritillaria raddeana* (Liliaceae) occurring with Alvanine, A-666 and Raddeamine, R-7. Cryst. Mp 235-236°.

Hydrochloride: Mp 174-175°.

Aslanov, Kh.A. *et al., Zh. Obshch. Khim.*, 1956, **26**, 579; *J. Gen. Chem. USSR (Engl. Transl.)*, 1956, **26**, 623

Alvanine A-666

$C_{26}H_{43}NO_3$ 417.631

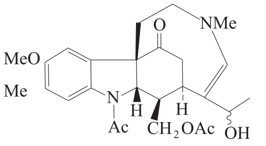
Prob. a steroidal alkaloid. Struct. unknown. Alkaloid from *Fritillaria raddeana* (Liliaceae). Cryst. Mp 185-187°. Co-occurs with Alvanidine, A-665 and Raddeamine, R-7.

Hydrochloride: Mp 163-165°.

Aslanov, Kh.A. *et al., Zh. Obshch. Khim.*, 1956, **26**, 579-583; *J. Gen. Chem. USSR (Engl. Transl.)*, 1956, **26**, 623

Alvimine A-667

1-Acetyl-17-(acetyloxy)-20,21-didehydro-19-hydroxy-10,11-dimethoxy-4-methyl-3,4-secocuran-3-one, 9CI
[82083-63-4]



Absolute configuration

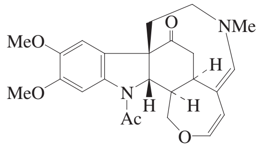
$C_{26}H_{34}N_2O_7$ 486.564

Alkaloid from bark of *Strychnos alvimiana* (Loganiaceae). Cryst. (EtOAc/hexane). Mp 124-126°. $[\alpha]_D^{20}$ +282 (c, 0.5 in EtOH).

Marini-Bettolo, G.B. *et al., An. Asoc. Quim. Argent.*, 1982, **70**, 263 (*isol, ir, uv, pmr, ms, struct*)

Alviminine A-668

[82083-62-3]



Probable Absolute Configuration

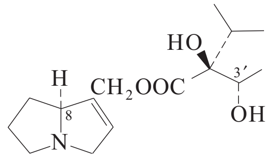
$C_{24}H_{28}N_2O_5$ 424.496

Tentative struct. Alkaloid from the bark of *Strychnos alvimiana* (Loganiaceae). Cryst. (EtOAc/hexane). Mp 103-106°.

Marini-Bettolo, G.B. *et al., An. Asoc. Quim. Argent.*, 1982, **70**, 263 (*isol, uv, pmr, cmr, ms, struct*)

Amabiline† A-669

[17958-43-9]



$C_{15}H_{25}NO_4$ 283.367

Amabiline and its stereoisomers are esters of Supinidine, S-644 with stereoisomers of 2,3-Dihydroxy-2-isopropylbutanoic acid. Alkaloid from *Cynoglossum amabile* dried whole plants and from whole plants of *Neatostema apulum* (Boraginaceae). Noncryst. $[\alpha]_D^{20}$ -7.1 (c, 2.02 in EtOH). Cryst. derivs. could not be obt.

N*-Oxide:* ***Amabiline*** **N*-oxide***
[145265-23-2]
$C_{15}H_{25}NO_5$ 299.366
Alkaloid from whole plants of *Neatostema apulum* (Boraginaceae). $[\alpha]_D$ -12 (c, 1.4 in EtOH).

8-Epimer: ***Cynaustine***
[17958-39-3]
$C_{15}H_{25}NO_4$ 283.367
Minor alkaloid from *Cynoglossum australe* dried plants (Boraginaceae). Pale-yellow gum. $[\alpha]_D^{20}$ +13.2 (c, 1.59 in EtOH). Ester of (+)-supinine with (-)-viridifloric acid.

▶ EK7792000

8-Epimer, picrate:
Yellow plates (EtOH). Mp 135-136°.

3′-Epimer: ***Supinine***
[551-58-6]
$C_{15}H_{25}NO_4$ 283.367
Alkaloid from *Heliotropium supinum* and *Heliotropium europaeum* (Boraginaceae). Shows antineoplastic props. Needles (Me_2CO). Mp 148-149° (146-147.5°). $[\alpha]_D$ -23.8 (EtOH). $[\alpha]_D$ -12.1 (c, 1.98 in EtOH). Log P 0.2 (calc).

▶ Hepatotoxin. WU2050000

3′-Epimer, $O^{3'}$*-Me,* N*-oxide:* ***Heleurine*** **N*-oxide***
[132886-10-3]
$C_{16}H_{27}NO_5$ 313.393
Alkaloid from aerial parts of *Heliotropium hirsutissimum* (Boraginaceae).

Gummy solid. $[\alpha]_D^{20}$ +19.5 (c, 0.55 in $CHCl_3$).

3′-Epimer, $O^{3'}$*-Me:* ***Heleurine****. Alkaloid C*†
[488-00-6]
$C_{16}H_{27}NO_4$ 297.394
Alkaloid from *Heliotropium indicum* and *Heliotropium europaeum* (Boraginaceae). Large transparent prisms. Sol. H_2O. Mp 67-68°. $[\alpha]_D^{16}$ -12 (c, 5.15 in EtOH). Discolours rapidly unless v. pure.

▶ EK7879200

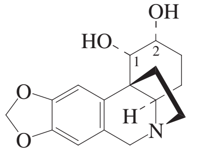
2′-Epimer: ***Heliovinine***
[84471-36-3]
$C_{15}H_{25}NO_4$ 283.367
Minor alkaloid from *Heliotropium curassavicum* (Boraginaceae). Gum. Probable struct. Obt. only as a mixt. with Coromandalinine and Curassavinine.

2′,3′-Diepimer: ***Coromandalinine***
[85798-06-7]
$C_{15}H_{25}NO_4$ 283.367
Probable struct. Obt. only as a mixt. with Heliovinine and Curassavinine. Minor alkaloid from *Heliotropium curassavicum* (Boraginaceae). Gum.

Men'shikov, G.P. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1949, **19**, 1382; *CA*, **44**, 3486 (*isol, Supinine*)
Culvenor, C.C.J. *et al., Aust. J. Chem.*, 1954, **7**, 287; 1967, **20**, 2499 (*Supinine, Amabiline, Cynaustine, Heleurine*)
Culvenor, C.C.J. *et al., Chem. Ind. (London)*, 1959, 20 (*synth, Supinine*)
Mattocks, A.R. *et al., Nature (London)*, 1968, **217**, 723 (*tox, Supinine*)
Šimánek, V. *et al., Coll. Czech. Chem. Comm.*, 1969, **34**, 1832 (*uv, Supinine*)
Culvenor, C.C.J. *et al., J.C.S.(C)*, 1971, 3653 (*cd*)
Mohanraj, S. *et al., Phytochemistry*, 1982, **21**, 1775 (*Coromandalinine, Heliovinine*)
Mackay, M.F. *et al., Acta Cryst. C*, 1985, **41**, 722-725 (*cryst struct, Supinine, Heleurine*)
Roeder, E. *et al., Phytochemistry*, 1992, **31**, 3613 (*Amabiline N-oxide*)
Constantinidis, T. *et al., Phytochemistry*, 1993, **32**, 1335 (*Heleurine N-oxide*)
Logie, C.G. *et al., Phytochemistry*, 1994, **37**, 43-109 (*rev, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SOW500

Amabiline† A-670

Crinan-1,2-diol, 9CI
[151204-56-7]



Absolute Configuration

$C_{16}H_{19}NO_4$ 289.33
Alkaloid from bulbs of *Crinum amabile* and *Crinum kirkii* (Amaryllidaceae). Mp 210° dec. $[\alpha]_D^{20}$ -32 (c, 0.3 in EtOH). λ_{max} 209 (log ε 4.13); 234 (log ε 3.49); 292 (log ε 3.61) (EtOH).

2-Epimer, O^2*-Ac:* ***Josephinine***
[157469-84-6]
$C_{18}H_{21}NO_5$ 331.368
Alkaloid from bulbs of *Brunsvigia josephinae* (Amaryllidaceae). Mp 230-232°. $[\alpha]_D^{22}$ -30.9 (c, 0.5 in EtOH).

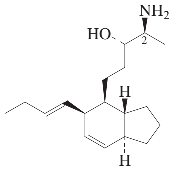
1,2-Diepimer: ***4a-Deoxycrinamabine****. 4a-Dehydroxycrinamabine*
[211234-46-7]
$C_{16}H_{19}NO_4$ 289.33
Alkaloid from the bulbs of *Crinum amabile*. Mp 208-210° dec. $[\alpha]_D^{29}$ +28 (c, 0.1 in MeOH). λ_{max} 205 (log ε 4.07); 237 (sh) (log ε 3.4); 289 (log ε 3.24) (MeOH).

1,2-Diepimer, 1,2-di-Ac: ***1-Epidemethoxybowdensine***
[184900-14-9]
$C_{20}H_{23}NO_6$ 373.405
Alkaloid from bulbs of *Brunsvigia orientalis*. Mp 96-98°. $[\alpha]_D^{22}$ +20 (c, 0.78 in $CHCl_3$).

Likhitwitayawuid, K. *et al., J. Nat. Prod.*, 1993, **56**, 1331-1338 (*isol, uv, ir, pmr, cmr, ms, struct*)
Viladomat, F. *et al., Phytochemistry*, 1994, **35**, 809-812; 1996, **43**, 1379-1384 (*Josephinine, 1-Epidemethoxybowdensine*)
Pearson, W.H. *et al., J.O.C.*, 1998, **63**, 3607-3617 (*synth*)
Pham, L.H. *et al., Phytochemistry*, 1998, **48**, 371-376 (*4a-Deoxycrinamabine*)
Machocho, A.K. *et al., Phytochemistry*, 2004, **65**, 3143-3149 (*isol*)

Amaminol A A-671

[261622-18-8]



Absolute Configuration

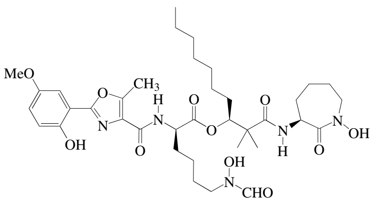
$C_{18}H_{31}NO$ 277.449
Isol. from an unidentified tunicate of the family Polyclinidae. Cytotoxic agent. Pale yellow oil. $[\alpha]_D^{24}$ -170.8 (c, 0.2 in MeOH).

2-Epimer: ***Amaminol B***
[261622-22-4]
$C_{18}H_{31}NO$ 277.449
Isol. from an unidentified tunicate of the family Polyclinidae. Cytotoxic agent. Pale yellow oil. $[\alpha]_D^{24}$ -112.4 (c, 0.2 in MeOH).

Sata, N.U. *et al., Tet. Lett.*, 2000, **41**, 489-492 (*isol, pmr, cmr*)
Kumpulainen, E.T.T. *et al., Org. Lett.*, 2007, **9**, 5043-5045 (*synth, abs config*)

Amamistatin A A-672

[225505-59-9]



Absolute Configuration

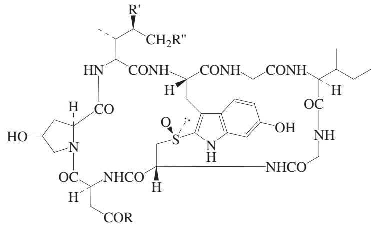
$C_{37}H_{55}N_5O_{11}$ 745.868
Prod. by *Nocardia asteroides* SCRC-A 2359. Antitumour and antiproliferative agent. Mast cell growth inhibitor. $[\alpha]_D^{26}$ -9.8 (c, 0.61 in MeOH). Related to Formobactin, F-130 and Nocobactin NA, N-267. λ_{max} 272 (ε 22000); 335 (ε 11000) (MeOH).

Demethoxy: ***Amamistatin B***
[225505-77-1]
$C_{36}H_{53}N_5O_{10}$ 715.842
Prod. by *Nocardia asteroides* SCRC-A 2359. Antitumour and antiproliferative agent. Mast cell growth inhibitor. $[\alpha]_D^{28}$ -8.2 (c, 0.47 in MeOH). λ_{max} 266 (ε 22000); 307 (ε 12000) (MeOH).

Yokokawa, F. *et al., Tetrahedron*, 2000, **56**, 3027-3034 (*synth*)
Kokubo, S. *et al., Tetrahedron*, 2000, **56**, 6435-6440 (*isol, uv, ir, pmr, cmr, abs config*)
Fennell, K.A. *et al., J.O.C.*, 2008, **73**, 1018-1024 (*synth*)

Amanitin† A-673

Amantin. Amatoxin



α-Amanitin	R = NH_2, R' = R'' = OH
β–Amanitin	R' = R'' = OH
γ-Amanitin	R = NH_2, R' = OH, R'' = H
ε-Amanitin	R = R' = OH, R'' = H
Amanullin	R =NH_2, R' = R'' = H
Amanullin acid	R = OH, R' = R'' = H

α-Amanitin [23109-05-9]
$C_{39}H_{54}N_{10}O_{14}S$ 918.98
Toxic constit. of *Amanita phalloides*. Also from *Amanita verna, Amanita bisporigera, Galerina autumnalis, Galerina marginata* and *Galerina venenata*. Needles. Sol. MeOH, H_2O. Mp 254-255° dec. $[\alpha]_D^{20}$ +191 (H_2O). λ_{max} 302 (MeOH) (Berdy).

▶ Systemic effects in humans by ingestion. Can cause hepatic necrosis, liver failure and death if untreated. Nephrotoxic. LD_{50} (mus, ipr) 0.1 mg/kg. Some human and exp. toxic effects are delayed (2-8 d after administration) *cf.* phallotoxins. Gastrointestinal effects occur 2-4 h after ingestion. BD6195000

Deoxy: ***Amaninamide***
[58311-65-2]
$C_{39}H_{54}N_{10}O_{13}S$ 902.981
Isol. from *Amanita virosa*. Lacks the OH group on the tryptophan ring.

β-Amanitin
1-L-Aspartic acid-α-amanitin, 9CI
[21150-22-1]
$C_{39}H_{53}N_9O_{15}S$ 919.965
Toxic constit. of several spp. of *Amanita*, notably *Amanita phalloides* and also

found in *Galerina autumnalis, Galerina venenata, Galerina marginata* and *Amanita bisporigera*. Cryst. (EtOH). Sol. H_2O, EtOH. Mp 300°. λ_{max} 302 (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 0.4 mg/kg. NJ8324000

Deoxy: ***Amanin**. 1-L-Aspartic acid-4-(2-mercapto-L-tryptophan)-α-amanitin, 9CI*
[21150-21-0]
$C_{39}H_{53}N_9O_{14}S$ 903.966
Constit. of *Amanita phalloides* toxin. Lacks the OH-group on the tryptophan ring.

▶ LD_{50} (mus, ipr) 0.5 mg/kg. NJ8326000

γ-Amanitin
3-(4-Hydroxy-L-isoleucine)-α-amanitin, 9CI
[21150-23-2]
$C_{39}H_{54}N_{10}O_{13}S$ 902.981
Constit. of *Amanita phalloides.*

▶ LD_{50} (mus, ipr) 0.2 mg/kg. NJ8323000

ϵ-Amanitin
*1-L-Aspartic acid-3-(*S*)-4-hydroxy-L-isoleucine-α-amanitin, 9CI*
[21705-02-2]
$C_{39}H_{53}N_9O_{14}S$ 903.966

▶ LD_{50} (mus, ipr) 0.3 mg/kg. NJ8325000

Amanullinic acid
1-L-Aspartic acid-3-isoleucine-α-amanitin, 9CI
[54532-45-5]
$C_{39}H_{53}N_9O_{13}S$ 887.966
Constit. of *Amanita phalloides.*

▶ LD_{50} (mus, ipr) >20 mg/kg. BD6093000

Amanullin [21803-57-6]
$C_{39}H_{54}N_{10}O_{12}S$ 886.981
Constit. of *Amanita phalloides.*

▶ LD_{50} (mus, ipr) >20 mg/kg. BD6200000

Deoxy: ***Proamanullin**. 2-L-Proline-3-isoleucine-α-amanitin*
[54532-46-6]
$C_{39}H_{54}N_{10}O_{11}S$ 870.982
Constit. of *Amanita phalloides*. Lacks the 4-hydroxyprolyl OH group.

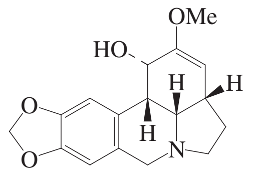
▶ LD_{50} >20mg/Kg (mus, ipr). BD6300000

[11030-71-0]

Wieland, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1967, **25**, 214 (*rev*)
Wieland, T. *et al., Annalen*, 1974, 1561; 1570; 1580; 1587 (*bibl, abs config*)
Yocum, R.R. *et al., Biochemistry*, 1978, **17**, 3786; 3790 (*isol, purifn, cryst struct*)
Wieland, T. *et al., Crit. Rev. Biochem.*, 1978, **5**, 185 (*rev*)
Buku, A. *et al., Experientia*, 1980, **36**, 33-34 (*Amaninamide*)
Wieland, T. *et al., Peptides of Poisonous Amanita Mushrooms*, Springer-Verlag, 1986, (*book*)
Michelot, D. *et al., Drug Metab. Drug Interact.*, 1988, **6**, 265 (*biol props*)
Shoham, G. *et al., J.A.C.S.*, 1989, **111**, 4791 (*cryst struct*)
Pehk, T. *et al., Magn. Reson. Chem.*, 1989, **27**, 173 (*pmr, conformn*)
Antkowiak, R. *et al., Alkaloids (Academic Press)*, 1991, **40**, 189 (*rev*)
Tagliaro, F. *et al., J. Chromatogr.*, 1991, **563**, 299 (*hplc*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1390
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AHI625

Amarbellisine A-674

[767356-23-0]

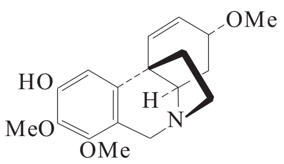


$C_{17}H_{19}NO_4$ 301.341
Alkaloid from the bulbs of *Amaryllis belladonna*. Needles (MeOH). Mp > 300°. $[\alpha]_D^{25}$ -39.2 (c, 0.7 in $CHCl_3$). λ_{max} 244 (log ϵ 2.9); 293 (log ϵ 2.9) (MeOH).

Evidente, A. *et al., Phytochemistry*, 2004, **65**, 2113-2118 (*isol, cd, pmr, cmr, ms*)

Amaryllisine A-675

[6874-70-0]



$C_{18}H_{23}NO_4$ 317.384
Alkaloid from *Amaryllis belladonna (Brunsvigia rosea)* (Amaryllidaceae). Prisms (MeOH). Mp 255-258° dec. $[\alpha]_D^{24}$ +2.4. $[\alpha]_{436}^{24}$ -6.6 (c, 0.27 in $CHCl_3$).

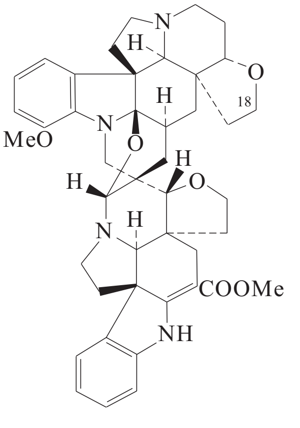
Ac: Mp 181-182°.

Me ether:
Fine prisms (cyclohexane). Mp 99-100°. $[\alpha]_D^{24}$ -16.4 (c, 1.6 in $CHCl_3$).

Burlingame, A.L. *et al., J.A.C.S.*, 1964, **86**, 4976 (*isol, uv, ir, pmr, ms, struct*)

Amataine A-676

Grandifoline†. *Subsessiline*†
[31148-60-4]



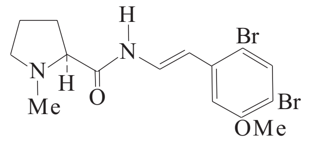
$C_{43}H_{48}N_4O_6$ 716.875
Alkaloid from the root bark of *Hedranthera (Callichilia) barteri* and *Voacanga chalotiana*, the stems of *Callichilia subsessilis* and the leaves of *Voacanga grandifolia* (Apocynaceae). Shows antimicrobial activity. Cryst. (hexane). Mp 216-221°. $[\alpha]_D^{26}$ -262 (c, 0.727 in $CHCl_3$).

18-Oxo: ***Subsessiline lactone**. 18-Oxoamataine. Alkaloid H*†
[59796-72-4]
$C_{43}H_{46}N_4O_7$ 730.859
Alkaloid from the leaves of *Voacanga thouarsii* (Apocynaceae). Cryst. (Me_2CO). Mp 237-239° dec. $[\alpha]_D$ -292.

Agwada, V. *et al., Helv. Chim. Acta*, 1970, **53**, 1567; 1977, **60**, 2830 (*isol, uv, ir, pmr, ms, ord, struct*)
Rolland, Y. *et al., Phytochemistry*, 1973, **12**, 2039 (*deriv*)
Gabetta, B. *et al., Fitoterapia*, 1974, **45**, 32; *CA*, **81**, 166291t (*isol*)
Rolland, Y. *et al., J.O.C.*, 1976, **41**, 3270 (*cmr, struct, deriv*)
Rolland, Y. *et al., Helv. Chim. Acta*, 1977, **60**, 2854 (*cd, ms, deriv*)
Villar, A. *et al., Planta Med.*, 1986, **52**, 556-557 (*activity*)

Amathamide A A-677

[99615-75-5]



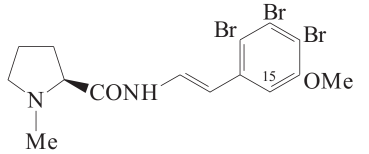
$C_{15}H_{18}Br_2N_2O_2$ 418.127
Alkaloid from the marine bryozoan *Amathia wilsoni*. Mp 189-190.5°.

(Z)-Isomer: ***Amathamide B***
[99615-76-6]
Alkaloid from *Amathia wilsoni*. Oil.

Blackman, A.J. *et al., Heterocycles*, 1985, **23**, 2829-2833 (*isol, ir, pmr, cmr, ms, cd, struct, abs config*)

Amathamide E A-678

[112515-28-3]



$C_{15}H_{17}Br_3N_2O_2$ 497.023
Alkaloid from the bryozoan *Amathia wilsoni*. Light yellow oil.

N*-Me:* ***Amathamide C***
[112515-26-1]
$C_{16}H_{19}Br_3N_2O_2$ 511.05
Alkaloid from *Amathia wilsoni* and *Amathia pinnata*. Pale yellow oil.

Dihydro: ***Amathamide D***
[112515-27-2]
$C_{15}H_{19}Br_3N_2O_2$ 499.039
Alkaloid from *Amathia wilsoni*. Light green oil.

(Z)-Isomer: ***Amathamide F***
[112515-29-4]

$C_{15}H_{17}Br_3N_2O_2$ 497.023
Alkaloid from *Amathia wilsoni*. Oil.

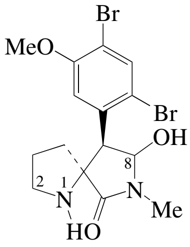
N-*Me, 15-methoxy:* ***Amathamide G***
[149355-72-6]
$C_{17}H_{21}Br_3N_2O_3$ 541.076
Alkaloid from *Amathia convoluta*. Oil.

Blackman, A.J. *et al., Aust. J. Chem.*, 1987, **40**, 1655-1662 (*isol, ir, pmr, cmr, ms, struct*)
Blackman, A.J. *et al., Aust. J. Chem.*, 1993, **46**, 401-405 (*Amathamide G*)

Amathaspiramide C

A-679

[226993-86-8]



$C_{15}H_{18}Br_2N_2O_3$ 434.127
Alkaloid from the marine bryozoan *Amathia wilsoni*. Amorph. solid. $[\alpha]_D^{25}$ -2 (c, 0.005 in MeOH). λ_{max} 215 (log ϵ 4.16); 289 (log ϵ 3.15); 294 (log ϵ 3.15) (MeOH).

N^1-*Me:* ***Amathaspiramide A***
[226993-84-6]
$C_{16}H_{20}Br_2N_2O_3$ 448.154
Alkaloid from *Amathia wilsoni*. Amorph. solid. $[\alpha]_D^{25}$ -3 (c, 0.004 in MeOH). λ_{max} 216 (log ϵ 4.2); 289 (log ϵ 3.34); 295 (log ϵ 3.36) (MeOH).

1,2-Didehydro: ***Amathaspiramide E***
[226993-88-0]
$C_{15}H_{16}Br_2N_2O_3$ 432.111
Alkaloid from *Amathia wilsoni*. Amorph. solid. $[\alpha]_D^{25}$ -21 (c, 0.002 in MeOH). λ_{max} 220 (log ϵ 4.13); 289 (log ϵ 3.17); 295 (log ϵ 3.17) (MeOH).

2-Oxo: ***Amathaspiramide D***
[226993-87-9]
$C_{15}H_{16}Br_2N_2O_4$ 448.11
Alkaloid from *Amathia wilsoni*. Amorph. solid. $[\alpha]_D^{25}$ -44 (c, 0.002 in MeOH). λ_{max} 215 (log ϵ 4.03); 289 (log ϵ 3.22); 295 (log ϵ 3.22) (MeOH).

2-Oxo, N^1-*Me:* ***Amathaspiramide B***
[226993-85-7]
$C_{16}H_{18}Br_2N_2O_4$ 462.137
Alkaloid from *Amathia wilsoni*. Amorph. solid. $[\alpha]_D^{25}$ -13 (c, 0.002 in MeOH). λ_{max} 208 (log ϵ 4.5); 310 (log ϵ 4.38); 436 (log ϵ 4.6) (MeOH).

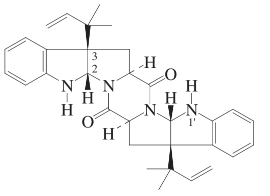
8-Epimer: ***Amathaspiramide F***
[226993-89-1]
$C_{15}H_{18}Br_2N_2O_3$ 434.127
Alkaloid from *Amathia wilsoni*. Amorph. solid. $[\alpha]_D$ -10 (c, 0.002 in MeOH). λ_{max} 214 (log ϵ 4.12); 290 (log ϵ 3.08); 296 (log ϵ 3.08) (MeOH).

Morris, B.D. *et al., J. Nat. Prod.*, 1999, **62**, 688-693 (*isol, uv, ir, pmr, cmr, ms*)
Hughes, C.C. *et al., Angew. Chem., Int. Ed.*, 2002, **41**, 4556-4559 (*Amathaspiramide F, synth*)
Sakaguchi, K. *et al., Org. Lett.*, 2008, **10**, 5449-5452 (*Amathaspiramide F, synth*)

Amauromine

A-680

FR 900220. WF 6237. Antibiotic FR 900220. Antibiotic WF 6237
[88360-87-6]



$C_{32}H_{36}N_4O_2$ 508.662
Diketopiperazine antibiotic. Isol. from *Amauroascus* sp. ATCC 20595 and *Penicillium nigricans* IMI 228669. Hypotensive vasodilator; gastric juice secretion inhibitor, calcium channel blocker. Prisms (EtOH). Sol. MeOH, Me_2CO, Py, $CHCl_3$; poorly sol. H_2O, hexane. Mp 156-158°. $[\alpha]_D^{23}$ -583 (c, 1 in $CHCl_3$). λ_{max} 245 (ϵ 11000); 300 (ϵ 4200) (EtOH) (Derep).
▸ LD_{50} (mus, ipr) 200 mg/kg. UQ3987000

2,3-Diepimer: ***Epiamauromine***
[143168-22-3]
$C_{32}H_{36}N_4O_2$ 508.662
Metab. from sclerotia of *Aspergillus ochraceus* NRRL 3519. Insect antifeedant, insecticide. Solid. Mp 134°. $[\alpha]_D$ -50 (c, 0.18 in $CHCl_3$). λ_{max} 215 (ϵ 100000); 243 (ϵ 100000); 300 (ϵ 40000) (MeOH) (Berdy).

2,3-Diepimer, $N^{1'}$-*Me:* **N-*Methylepiamauromine***
[143086-28-6]
$C_{33}H_{38}N_4O_2$ 522.689
Metab. from the sclerotia of *Aspergillus ochraceus* NRRL 3519. Insect antifeedant, insecticide. $[\alpha]_D$ -29.1 (c, 0.46 in $CHCl_3$). λ_{max} 214 (ϵ 25000); 244 (ϵ 12500); 303 (ϵ 6400) (MeOH) (Berdy).

Stereoisomer: ***Nigrifortine***
[97859-13-7]
$C_{32}H_{36}N_4O_2$ 508.662
Metab. of *Penicillium nigricans*. Stereochem. not determined. May be identical with Amauromine or Epiamauromine.

Takase, S. *et al., J. Antibiot.*, 1984, **37**, 1320-1323 (*isol, props*)
Laws, I. *et al., Phytochemistry*, 1985, **24**, 1395-1397 (*Nigrifortine*)
Takase, S. *et al., Tetrahedron*, 1985, **41**, 3037-3048; 1986, **42**, 5887-5894 (*cryst struct, synth*)
De Guzman, F.S. *et al., J. Nat. Prod.*, 1992, **55**, 931-939 (*Epiamauromine, N-Methylepiamauromine*)
Marsden, S.P. *et al., J.A.C.S.*, 1994, **116**, 11143-11144 (*synth*)
Depew, K.M. *et al., J.A.C.S.*, 1999, **121**, 11953-11963 (*synth*)

Ambaline

A-681

$C_{38}H_{42}N_2O_{10}$ 686.757
Struct. unknown. Alkaloid from *Pycnarrhena manillensis*. Mp 123° Mp 265° (as dihydrochloride). $[\alpha]_D$ +143 ($CHCl_3$). Nonphenolic.

Quibilan, G.Q. *et al., CA*, 1934, **28**, 4735^2 (*isol*)

Ambalinine

A-682

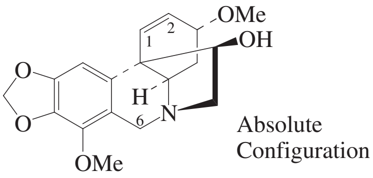
$C_{18}H_{21}NO_3$ 299.369
Struct. unknown. Nonphenolic, conts. 1 *N*-Me and 1 *O*Me group. Alkaloid from *Pycnarrhena manillensis*. Mp 203-204° Mp 238° (as picrate).

Villanos, M.I. *et al., CA*, 1936, **30**, 4171^7 (*isol*)

Ambelline

A-683

[3660-62-6]



$C_{18}H_{21}NO_5$ 331.368
C-12 config. incorr. given as 12*S*- in CAS. Alkaloid of *Brunsvigia rosea* (*Amaryllis belladonna*) and many other spp. in the Amaryllidaceae. Cytotoxic to P-388 sarcoma cells *in vitro*, shows no activity *in vivo*. Weak transient hypotensive agent and cardiac stimulant. Epinephrine potentiator, respiratory paralytic. Sol. MeOH, $CHCl_3$. Mp 260-261° (254-256°). $[\alpha]_D^{22}$ +81 (c, 0.56 in $CHCl_3$). $[\alpha]_D^{25}$ -13.6 (c, 0.11 in MeOH). λ_{max} 213 (log ϵ 4.6); 244 (sh) (log ϵ 3.64); 286 (log ϵ 3.24) (MeOH).
▸ Toxic, LD_{50} (mus, scu) 5 mg/kg.

Hydrochloride: Mp 227-230° dec.

Perchlorate: Mp 200° dec.

Ac: ***11-O-Acetylambelline***
[98983-14-3]
$C_{20}H_{23}NO_6$ 373.405
Alkaloid from bulbs of *Brunsvigia josephinae* (Amaryllidaceae). Mp 80-82°. $[\alpha]_D^{22}$ -23.5 (c, 0.59 in $CHCl_3$).

*11-*O*-(3-Pyridinecarbonyl):* ***Filifoline***†. *11-*O*-Nicotinoylambelline*
$C_{24}H_{24}N_2O_6$ 436.463
Alkaloid from the bulbs of *Nerine filifolia*. Powder. Mp 191-193°. $[\alpha]_D^{20}$ +12 (c, 0.85 in MeOH). λ_{max} 280 (log ϵ 5.93) (EtOH).

1β,2β-Epoxide: ***1,2-Epoxyambelline***
[93771-88-1]
$C_{18}H_{21}NO_6$ 347.367
Alkaloid from *Crinum latifolium* (Amaryllidaceae). Prisms (Me_2CO). Mp 245-246°. $[\alpha]_D^{22}$ +22.4 (c, 0.32 in $CHCl_3$).

1β,2β-Epoxide, Ac: ***11-O-Acetyl-1,2-epoxyambelline***
[93771-89-2]
$C_{20}H_{23}NO_7$ 389.404
Alkaloid from *Ammocharis tinneana*. Needles (Me_2CO). Mp 201-203° (195-197°).

Dihydro: ***Dihydroambelline***
$C_{18}H_{23}NO_5$ 333.383
Isol. from *Nerine crispa* (Amaryllidaceae). Mp 198-199°. $[\alpha]_D^{24}$ -12.6 (c, 0.5 in $CHCl_3$).

6α-Hydroxy: ***Crinafoline***
[106534-56-9]

$C_{18}H_{21}NO_6$ 347.367
Alkaloid from the mature fruits of *Crinum latifolium* (Amaryllidaceae). Has antitumour props. Microcryst. (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 234-237°. $[\alpha]_D^{28}$ +44.7 (c, 0.35 in MeOH). 12-Config. incorrectly given as 12*S*- in CAS.

6α-Hydroxy, di-Ac:
Prisms ($MeOH/Me_2CO$). Mp 214-215°.

6α-Hydroxy, N-*Me:*
$C_{19}H_{24}NO_5^{\oplus}$ 346.402
Straw-coloured solid (as iodide). Mp 262-265° dec.(iodide).

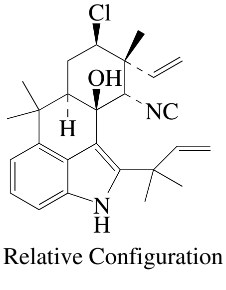
3-Epimer: ***Brunsbelline***
[171119-08-7]
$C_{18}H_{21}NO_5$ 331.368
Alkaloid from the bulbs of *Brunsvigia josephinae*. Mp 226-228°. $[\alpha]_D^{22}$ -97.8 (c, 0.1 in EtOH).

Stereoisomer, 1,2-epoxide: ***Cavinine***
[58189-38-1]
$C_{18}H_{21}NO_6$ 347.367
Alkaloid from *Hippeastrum puniceum* (Amaryllidaceae). Identified by ms only and assigned the same plane struct. as 1,2-Epoxyambelline without assignment of stereochem. May be identical with 1,2-Epoxyambelline.

Mason, L.H. *et al., J.A.C.S.*, 1955, **77**, 1253-1256 (*isol, uv, ir*)
Döpke, W. *et al., Naturwissenschaften*, 1962, **49**, 469 (*Dihydroambelline*)
Naegeli, P. *et al., J.O.C.*, 1963, **28**, 206-210 (*ir, pmr, struct*)
Duffield, A.M. *et al., J.A.C.S.*, 1965, **87**, 4902-4912 (*ms*)
Samuel, E.H.S. *et al., Org. Mass Spectrom.*, 1975, **10**, 427-431 (*Cavinine*)
Roques, R. *et al., Acta Cryst. B*, 1976, **32**, 1394-1398 (*cryst struct*)
Ghosal, S. *et al., J. Chem. Res., Synop.*, 1984, 232-233; 1986, 312-313 (*Epoxyambelline, Crinafoline*)
Viladomat, F. *et al., Phytochemistry*, 1994, **35**, 809-812 (*isol, cd, pmr, cmr, ms*)
Viladomat, F. *et al., Phytochemistry*, 1995, **40**, 961-965 (*11-O-Acetylambelline, Brunsbelline*)
Pham, L.H. *et al., Phytochemistry*, 1998, **48**, 371-376 (*isol, cd, uv, pmr, cmr, ms*)
Machocho, A. *et al., Phytochemistry*, 1999, **51**, 1185-1191 (*Epoxyambelline, O-Acetylepoxyambelline*)
Nair, J.J. *et al., Phytochemistry*, 2005, **66**, 373-382 (*Filifoline*)

Ambiguine B isonitrile A-684

A 89271C. Antibiotic A 89271C
[138630-60-1]



Relative Configuration

$C_{26}H_{31}ClN_2O$ 422.996
Alkaloid from the terrestrial blue-green alga *Fischerella ambigua*, also from *Hapalosiphon hibernicus* and *Westrellopsis prolifica*. Amorph. solid. $[\alpha]_D$ -44.3 (c, 0.1 in MeOH). λ_{max} 223 (ϵ 40700); 281 (ϵ 9400); 291 (ϵ 7700) (MeOH).

Deoxy: ***Ambiguine A isonitrile****. A 89271B. Antibiotic A 89271B*
[138630-59-8]
$C_{26}H_{31}ClN_2$ 406.997
From the terrestrial blue-green algae *Fischerella ambigua* and *Hapalosiphon hibernicus*, also *Westrellopsis prolifica*. Needles (hexane/CH_2Cl_2). Mp > 300° dec. $[\alpha]_D$ -37 (c, 0.1 in MeOH). λ_{max} 225 (ϵ 32400); 282 (ϵ 7600); 295 (sh) (ϵ 6500) (MeOH).

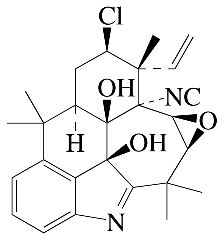
Dechloro: ***Ambiguine C isonitrile****. A 89271E. Antibiotic A 89271E*
[138630-61-2]
$C_{26}H_{32}N_2O$ 388.552
From *Fischerella ambigua*. Amorph. solid. $[\alpha]_D$ -9.5 (c, 0.1 in MeOH). λ_{max} 223 (ϵ 36000); 281 (ϵ 8400); 291 (ϵ 6800) (MeOH).

Dechloro, deoxy: ***Ambiguine H isonitrile***
$C_{26}H_{32}N_2$ 372.552
From a *Fischerella* sp. Amorph. solid. $[\alpha]_D^{25}$ -65 (c, 0.51 in MeOH). λ_{max} 222 (log ϵ 4.38); 282 (log ϵ 3.72); 291 (log ϵ 3.62) (MeOH).

Smitka, T.A. *et al., J.O.C.*, 1992, **57**, 857-861 (*isol, cd, uv, ir, pmr, cmr*)
Raveh, A. *et al., J. Nat. Prod.*, 2007, **70**, 196-201 (*isol, pmr, cmr*)

Ambiguine D isonitrile A-685

A 89271A. Antibiotic A 89271A
[138666-15-6]



Relative Configuration

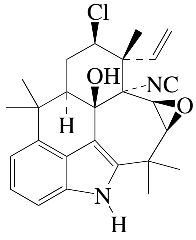
$C_{26}H_{29}ClN_2O_3$ 452.979
Alkaloid from the terrestrial blue-green algae *Fischerella ambigua* and *Westiellopsis prolifica*. Cryst. (MeOH aq.). Mp > 300° dec. $[\alpha]_D$ -30.3 (c, 0.1 in MeOH). λ_{max} 227 (ϵ 13900); 301 (ϵ 2170) (MeOH).

Dechloro: ***Ambiguine J isonitrile***
$C_{26}H_{30}N_2O_3$ 418.535
From a *Fischerella* sp. Amorph. solid. $[\alpha]_D^{25}$ -32 (c, 0.1 in MeOH). λ_{max} 222 (log ϵ 3.68); 270 (log ϵ 2.97); 308 (log ϵ 2.78) (MeOH).

Smitka, T.A. *et al., J.O.C.*, 1992, **57**, 857-861 (*isol, cd, uv, ir, pmr, cmr, cryst struct*)
Raveh, A. *et al., J. Nat. Prod.*, 2007, **70**, 196-201 (*isol, pmr, cmr*)

Ambiguine E isonitrile A-686

A 89271D. Antibiotic A 89271D
[138666-16-7]



Relative Configuration

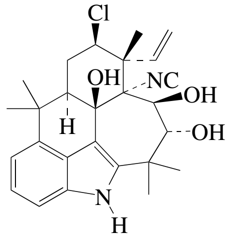
$C_{26}H_{29}ClN_2O_2$ 436.98
Alkaloid from the terrestrial blue-green algae *Fischerella ambigua*, *Hapalosiphon hibernicus* and *Westiellopsis prolifica*. Needles (hexane/CH_2Cl_2). Mp > 300° dec. $[\alpha]_D$ -59.7 (c, 0.1 in MeOH). λ_{max} 223 (ϵ 36000); 272 (ϵ 7100); 279 (ϵ 6800) (MeOH).

Dechloro: ***Ambiguine I isonitrile***
$C_{26}H_{30}N_2O_2$ 402.535
From a *Fischerella* sp. Amorph. solid. $[\alpha]_D^{25}$ -39 (c, 0.29 in MeOH). λ_{max} 222 (log ϵ 4.04); 282 (log ϵ 3.69); 286 (log ϵ 3.67) (MeOH).

Smitka, T.A. *et al., J.O.C.*, 1992, **57**, 857-861 (*isol, cd, uv, ir, pmr, cmr*)
Raveh, A. *et al., J. Nat. Prod.*, 2007, **70**, 196-201 (*isol, pmr, cmr*)

Ambiguine F isonitrile A-687

A 89271F. Antibiotic A 89271F
[138630-62-3]



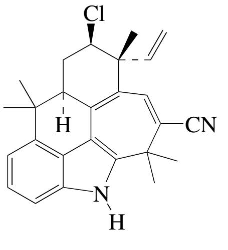
Relative Configuration

$C_{26}H_{31}ClN_2O_3$ 454.995
Alkaloid from the terrestrial blue-green alga *Fischerella ambigua*. Amorph. solid. $[\alpha]_D$ -18.2 (c, 0.1 in MeOH). λ_{max} 224 (ϵ 36000); 280 (ϵ 7200); 290 (ϵ 5500) (MeOH).

Smitka, T.A. *et al., J.O.C.*, 1992, **57**, 857 (*isol, uv, ir, pmr, cmr, cd, struct*)

Ambiguine G nitrile A-688

[213911-41-2]

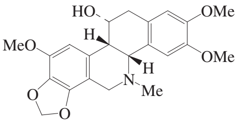


$C_{26}H_{27}ClN_2$ 402.965
Isol. from the blue-green alga *Hapalosiphon delicatulus.* $[\alpha]_D$ +138.3 (c, 0.6 in $CHCl_3$). λ_{max} 230 (ϵ 32400); 274 (ϵ 13900); 390 (ϵ 6750) (MeOH).

Huber, U *et al., J. Nat. Prod.*, 1998, **61**, 1304-1306 (*isol, uv, ir, pmr, cmr, ms*)

Ambinine A-689

[96935-26-1]



Absolute Configuration

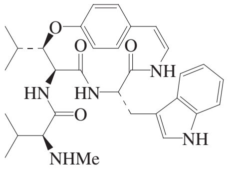
$C_{23}H_{27}NO_6$ 413.469
Minor alkaloid from the stem tuber of *Corydalis ambigua* (Papaveraceae). Prisms (EtOH). Mp 218-219°. $[\alpha]_D^{22}$ -106 (c, 1.3 in $CHCl_3$).

Hydrobromide: [132296-33-4]
Fine needles (EtOH). Mp 199-202°.

Cui, Z. *et al., Yaoxue Xuebao*, 1984, **19**, 904; *CA*, **103**, 19853x (*isol, uv, ir, pmr, cmr, ms, struct*)
Cui, Z. *et al., J. Nat. Prod.*, 1990, **53**, 1182 (*abs config, cd, cryst struct*)
Hanaoka, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 242 (*synth*)

Americine A-690

N-*[7-(1*H*-Indol-3-ylmethyl)-3-(1-methylethyl)-5,8-dioxo-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]-3-methyl-2-(methylamino)butanamide, 9CI*
[18867-84-0]



Absolute Configuration

$C_{31}H_{39}N_5O_4$ 545.68
Alkaloid from the root bark of *Ceanothus americanus* (New Jersey tea) (Rhamnaceae). Mp 135.5-137°. $[\alpha]_D^{20}$ -198 (c, 0.51 in MeOH).

N-*Me:* ***N-Methylamericine****. 5-β-Indolylmethyl-8*N-*(*N,N-*dimethylvalyl)-9-isopropylphencyclopeptine*
[70403-89-3]
$C_{32}H_{41}N_5O_4$ 559.707
Alkaloid from *Ceanothus integerrimus* and *Ceanothus sanguineus.* Mp 233° (229°).

Klein, F.K. *et al., J.A.C.S.*, 1968, **90**, 2398-2404 (*isol, uv, ir, pmr, ms, struct*)
Lagarias, J.C. *et al., J. Nat. Prod.*, 1979, **42**, 220-227; 663-668 (*N-Me*)

Amianthine A-691

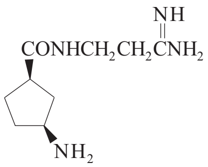
$C_{27}H_{41}NO_2$ 411.626
Steroidal alkaloid. Struct. unknown. Alkaloid from *Amianthium muscaetoxicum* (*Zygadenus muscaetoxicum*) (Liliaceae). Long prisms (Me_2CO). Mp 251-253° dec. $[\alpha]_D^{20}$ -87 (c, 0.173 in $CHCl_3$). pK_a 9.7.
Tertiary base contg. conjugated CO and acylable OH gps.

Ac: Mp 206-207° dec.

Neuss, N. *et al., J.A.C.S.*, 1953, **75**, 2772-2773 (*isol*)

Amidinomycin A-692

N-*(2-Amidinoethyl)-3-aminocyclopentanecarboxamide. Myxoviromycin*
[3572-60-9]



$C_9H_{18}N_4O$ 198.267
Prod. by *Streptomyces flavochromogenes.* Antifungal antiviral agent. Antineoplastic antibiotic. Sol. H_2O, EtOH, MeOH; poorly sol. butanol, hexane. Log P -2.26 (uncertain value) (calc). λ_{max} 205 (ϵ 4460) (0.1*N* HCl) (Derep). λ_{max} 219 (ϵ 1580) (0.1*N* NaOH) (Derep). λ_{max} 212 (ϵ 1170) (pH 3 H_2O) (Derep). λ_{max} 212 (E1%/1cm 59) (H_2O) (Berdy). λ_{max} 205 (E1%/1cm 225) (HCl) (Berdy). λ_{max} 219 (E1%/1cm 79) (NaOH) (Berdy).

▶ LD_{50} (mus, orl) 140 mg/kg, LD_{50} (mus, ivn) 18 mg/kg, LD_{50} (mus, ipr) 200 mg/kg. GY2555000

Sulfate:
Plates or needles (MeOH aq.). Mp 285-288° dec. $[\alpha]_D^{21}$ -3.9 (c, 3 in H_2O).

[19946-52-2]

Nakamura, S. *et al., Chem. Pharm. Bull.*, 1961, **9**, 641 (*synth, struct*)
Nakamura, S. *et al., J. Antibiot., Ser. A*, 1961, **14**, 103 (*isol, struct*)
Katsube, J. *et al., Chem. Pharm. Bull.*, 1968, **16**, 232 (*synth, ir, pmr*)
Allan, R.D. *et al., Aust. J. Chem.*, 1979, **32**, 2517 (*synth, struct*)
Kaneda, M. *et al., J. Antibiot.*, 1980, **33**, 778 (*cryst struct, abs config*)
Sapse, A.M. *et al., J. Biomol. Struct. Dyn.*, 1993, **10**, 709 (*conformn*)
Chenevert, R. *et al., Chem. Lett.*, 1994, 93 (*synth, abs config*)

2-Amino-12 methyl-1,3,12-tetradecanetriol A-693

$H_3CCH_2C(OH)(CH_3)(CH_2)_8$-$CH(OH)CH(NH_2)CH_2OH$

$C_{15}H_{33}NO_3$ 275.431

N-*Hydroxy,* N-*nitroso: 2-(Hydroxynitrosoamino)-12-methyl-1,3,12-tetradecanetriol, 9CI.* ***Nitrosostromelin***
[182064-61-5]
$C_{15}H_{32}N_2O_5$ 320.428
Prod. by a *Streptomyces* sp. Stromelysin inhibitor.

U.K. Pat., 1996, 2 297 324; *CA*, **125**, 245813v (*isol*)

2-Aminoacetophenone, 8CI A-694

2-Amino-1-phenylethanone, 9CI. Phenacylamine. Phenomydrol. Benzoylmethylamine. (Aminoacetyl)benzene
[613-89-8]
$PhCOCH_2NH_2$

C_8H_9NO 135.165
Component of tortilla aroma and of other corn flour products. Constit. of *Castanopsis cuspidata* and *Vitis* sp. Aroma threshold 0.2 ppb in H_2O.

▶ Exp. reprod. effects. AM5775000

Hydrochloride: [5468-37-1]
Needles (Me_2CO/EtOH). Mp 188°.

▶ AM5940000

Oxime:
$C_8H_{10}N_2O$ 150.18
Mp 140°.

2,4-Dinitrophenylhydrazone: Mp 221°.

Di-Et ketal:
$C_{12}H_{19}NO_2$ 209.288
Liq. $Bp_{0.5}$ 68°.

N-*Formyl:* [73286-37-0]
$C_9H_9NO_2$ 163.176
Cryst. (Me_2CO/hexane). Mp 80-82°.

N-*Ac:* [1846-33-9]
$C_{10}H_{11}NO_2$ 177.202
Mp 85°.

N-*Benzoyl: 2-(Benzoylamino)acetophenone.* N-*Phenacylbenzamide.* ***Muricatisine***
[4190-14-1]
$C_{15}H_{13}NO_2$ 239.273
Alkaloid from *Oxytropis muricata* and *Oxytropis puberula*. Cryst. (EtOH). Mp 122-124°.

N-*Me: α-Methylaminoacetophenone*
[35534-19-1]
$C_9H_{11}NO$ 149.192
Yellow oil.

N-*Me; hydrochloride:* [23826-47-3]
Plates. Mp 219° dec.

N-*Me,* N-*Ac:*
$C_{11}H_{13}NO_2$ 191.229
Mp 156°.

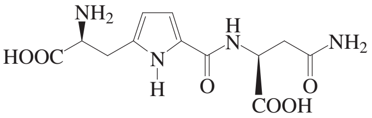
N,N-*Di-Me: 2-(*N,N-*Dimethylamino)acetophenone*
[3319-03-7]
$C_{10}H_{13}NO$ 163.219
Isol. from *Desmodium gangeticum*. Liq. Bp_{20} 130-132°.

[25384-14-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 46D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 867A (*nmr*)
Tiffeneau, M. *et al., Bull. Soc. Chim. Fr.*, 1931, **49**, 1761 (*rev*)
Stalham, F.S. *et al., J.C.S.*, 1951, 213 (*synth*)
Chapman, N.B. *et al., J.C.S.*, 1963, 1385 (*synth, deriv*)
Tanaka, H. *et al., CA*, 1971, **75**, 147849 (*struct*)
Ghosal, S. *et al., Planta Med.*, 1972, **22**, 434 (*isol, deriv*)
Bellamy, L.J. *et al., Spectrochim. Acta A*, 1972, **28**, 1869 (*ir*)
Yamaguchi, K. *et al., J. Agric. Food Chem.*, 1979, **27**, 847 (*isol*)
Muchowski, J.M. *et al., J.O.C.*, 1986, **51**, 3374 (*N-formyl*)
Abdalla, G.M. *et al., J. Het. Chem.*, 1987, **24**, 297 (*synth, ir, pmr*)
Yamagama, C. *et al., Aust. J. Chem.*, 1989, **42**, 463 (*N-15 nmr*)
Baumstark, A.L. *et al., Chem. Comm.*, 1989, 767 (*O-17 nmr*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1994, **42**, 1-2 (*occur, anal*)

Shure, K.B. *et al., J. Agric. Food Chem.*, 1994, **42**, 350 (*isol*)
Demeuov, N.B. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1998, **34**, 484-485 (*Muricatisine*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AHR250

α-Amino-5-[[(2-aminocarbonyl-1-carboxyethyl)amino]carbonyl]-2-pyrrolepropanoic acid, 9CI A-695



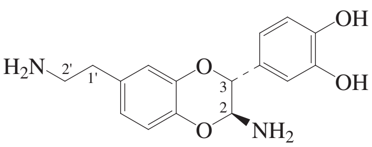
$C_{12}H_{16}N_4O_6$ 312.282

Minor metab. of *Pantoea agglomerans* (formerly *Erwinia herbicola*). λ_{max} 200 (ϵ 6440); 220 (sh) (ϵ 2994); 275 (ϵ 10890) (H_2O).

Jin, M. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 2898-2901; 2902-2905 (*isol, pmr, cmr, ms*)

2-Amino-6-(2-aminoethyl)-3-(3,4-dihydroxyphenyl)-1,4-benzodioxan A-696

2-Amino-3-(3,4-dihydroxyphenyl)-2,3-dihydro-1,4-benzodioxin-6-ethanamine



$C_{16}H_{18}N_2O_4$ 302.329

Dimer of Dopamine, D-920.

(2*S*,3*R*)-*form*

N,N′-*Ac:*

$C_{20}H_{22}N_2O_6$ 386.404

Isol. from the cast-off shells of the cicada *Cryptotympana* sp. Component of Zentai. Yellow powder. Mp 115-120°. $[\alpha]_D$ +28.2 (c, 1 in MeOH).

*1′,2′-Didehydro(*E*-),* N,N′-*di-Ac:*

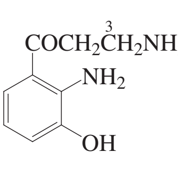
$C_{20}H_{20}N_2O_6$ 384.388

Isol. from the cast-off shells of *Cryptotympana pustulata*. Yellow powder. $[\alpha]_D^{25}$ +33.8 (c, 0.1 in MeOH). λ_{max} 282 (log ϵ 4.32) (MeOH).

Noda, N. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1749-1752 (*isol, pmr, cmr*)
Xu, M.-Z. *et al., Bioorg. Med. Chem.*, 2006, **14**, 7826-7834 (*deriv*)

3-Amino-1-(2-amino-3-hydroxyphenyl)-1-propanone A-697

2′,3-Diamino-3′-hydroxypropiophenone. 2-Amino-3-(3-aminopropanoyl)phenol. 3-Hydroxykynuramine



$C_9H_{12}N_2O_2$ 180.206

N^3-Ac: ***Erebusinone***. *Eribusinone*

[325477-44-9]

[194615-13-9]

$C_{11}H_{14}N_2O_3$ 222.243

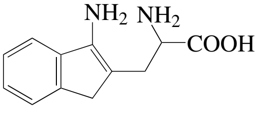
Isol. from the sponge *Isodictya erinacea*. Yellow solid. λ_{max} 238 (ϵ 1240); 372 (ϵ 180) (MeOH).

Moon, B. *et al., Tetrahedron*, 2000, **56**, 9057-9062 (*Erebusinone*)

2-Amino-3-(3-amino-1*H*-inden-2-yl)propanoic acid A-698

*α,3-Diamino-1*H*-indene-2-propanoic acid, 9CI. 3-(3-Amino-1*H*-inden-2-yl)alanine.* ***Cycasindene***

[192801-71-1]



$C_{12}H_{14}N_2O_2$ 218.255

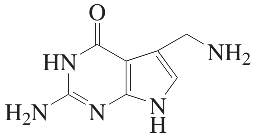
Constit. of the seeds of *Cycas revoluta* (Cycadaceae). Microcryst.

Pan, M. *et al., Phytochemistry*, 1997, **45**, 517-519 (*isol, pmr, cmr*)

2-Amino-5-(aminomethyl)pyrrolo[2,3-*d*]pyrimidin-4(3*H*)-one, 9CI A-699

7-Aminomethyl-7-deazaguanine. Pre-Q1 base

[69251-45-2]



$C_7H_9N_5O$ 179.181

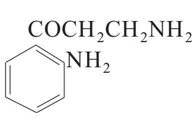
Isol. from *Escherichia coli* tRNA. Biosynthetic precursor of Queuine, Q-9. Solid; cryst. + $2H_2O$ (as hydrochloride). Mp 220-225° dec. (hydrochloride).

Ohgi, T. *et al., Chem. Lett.*, 1979, 1283 (*synth, ir, ms, pmr, uv, derivs*)
Okada, N. *et al., J. Biol. Chem.*, 1979, **254**, 3067 (*isol, synth*)
Farkas, W.R. *et al., Biochim. Biophys. Acta*, 1984, **781**, 64 (*metab*)
Akimoto, H. *et al., J.C.S. Perkin 1*, 1988, 1637 (*synth, ir, pmr, bibl*)
Klepper, F. *et al., Helv. Chim. Acta*, 2005, **88**, 2610-2616 (*synth, ir, pmr, cryst struct*)

3-Amino-1-(2-aminophenyl)-1-propanone, 9CI A-700

2′,3-Diaminopropiophenone. ***Kynuramine***

[363-36-0]



$C_9H_{12}N_2O$ 164.207

Found in rat brains, and derived from tryptophan. Liq.

Hydrochloride: Mp 185-187° dec.

Picrate: Mp 176-177° dec.

N^3-*Ac:* **N^3-*Acetylkynuramine***

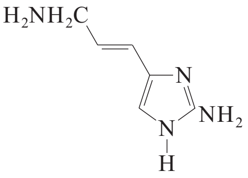
$C_{11}H_{14}N_2O_2$ 206.244

Prod. by the marine-derived *Janibacter limosus* Hel 1. Light yellow oil. λ_{max} 202 (log ϵ 4.21); 227 (log ϵ 4.31); 362 (log ϵ 3.61) (MeOH). λ_{max} 208 (log ϵ 4.3); 227 (log ϵ 4.31); 255 (log ϵ 3.77); 360 (log ϵ 3.68) (MeOH/NaOH).

Butenandt, A. *et al., Z. Naturforsch., B*, 1953, **86**, 454 (*synth, pharmacol*)
Seiler, N. *et al., CA*, 1971, **74**, 39005 (*ms*)
Gal, E.M. *et al., J. Neurochem.*, 1978, **30**, 607 (*occur*)
Asolkar, R.N. *et al., J. Antibiot.*, 2004, **57**, 17-23 (*N^3-Acetylkynuramine*)

2-Amino-4-(3-amino-1-propenyl)-1*H*-imidazole A-701

*4-(3-Amino-1-propenyl)-1*H*-imidazol-2-amine, 9CI. 3-(2-Amino-1*H*-imidazol-4-yl)-2-propen-1-amine. 3-Amino-1-(2-aminoimidazolyl)-1-propene*



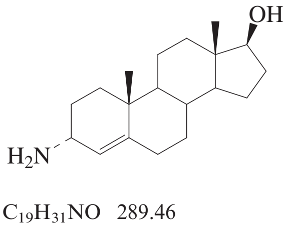
$C_6H_{10}N_4$ 138.172

(*E*)-*form* [140381-65-3]

Alkaloid from *Agelas oroides*, *Ptilocaulis walpersi* and *Teichaxinella morchella*. Light brown oil. λ_{max} 276 (ϵ 8790) (MeOH) (Derep).

Wright, A.E. *et al., J. Nat. Prod.*, 1991, **54**, 1684-1686 (*isol, uv, pmr, cmr*)
Tasdemir, D. *et al., Bioorg. Med. Chem.*, 2008, **15**, 6834-6845 (*isol, pmr, cmr*)

3-Aminoandrost-4-en-17-ol A-702



$C_{19}H_{31}NO$ 289.46

(3α,17β)-*form*

N-*Carbamoyl:* ***3-Ureidoandrost-4-en-17-ol***

$C_{20}H_{32}N_2O_2$ 332.485

Alkaloid from the musk of *Moschus moschiferus*. Amorph. powder. Mp 210-212°. $[\alpha]_D^{25}$ +250 (c, 0.02 in MeOH). Dec. at 215°.

17-Ketone, N-*carbamoyl:* ***3-Ureidoandrost-4-en-17-one***

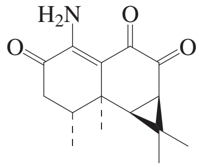
$C_{20}H_{30}N_2O_2$ 330.469

Alkaloid from the musk of *Moschus moschiferus*. Amorph. powder. Mp

220-223°. $[\alpha]_D^{25}$ +115 (c, 0.002 in MeOH).

Oh, S.-R. *et al., Chem. Pharm. Bull.*, 2002, **50**, 663-664 (*isol, pmr, cmr*)

1-Amino-1(10)-aristolene-2,8,9-trione A-703



$C_{15}H_{19}NO_3$ 261.32

ent-form

Lepidamine

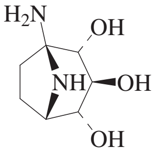
[609332-21-0]

Prod. by *Russula lepida*. Pale yellow oil. $[\alpha]_D$ +125 (c, 0.36 in $CHCl_3$). λ_{max} 242 ; 409 (Et_2O).

Tan, J. *et al., Helv. Chim. Acta*, 2003, **86**, 307-309 (*isol, pmr, cmr, ms*)

1-Amino-8-azabicyclo[3.2.1]octane-2,3,4-triol A-704

1-Amino-2,3,4-trihydroxynortropane



$C_7H_{14}N_2O_3$ 174.199

(1*S*,2*R*,3*R*,4*S*)-*form*

Calystegine N₁

[177794-03-5]

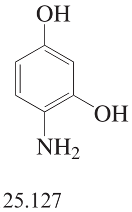
Alkaloid from *Hyoscyamus niger* (Solanaceae). Shows glycosidase inhibitory activity. $[\alpha]_D$ +59.4 (c, 0.2 in H_2O).

Asano, N. *et al., Carbohydr. Res.*, 1996, **284**, 169-178 (*isol, pmr, cmr, activity*)
Bekkouche, K. *et al., Phytochemistry*, 2001, **58**, 455-462 (*ms, occur*)
Biastoff, S. *et al., Alkaloids (Academic Press)*, 2007, **64**, 49-102 (*rev*)

4-Amino-1,3-benzenediol, 9CI A-705

4-Aminoresorcinol, 8CI. 2,4-Dihydroxyaniline

[13066-95-0]



$C_6H_7NO_2$ 125.127

Used in hair dyes. pK_{a1} 7.91; pK_{a2} 9.16; pK_{a3} 11.24 (20°). Unstable.

3-Me ether: 4-Amino-3-methoxyphenol
[61638-01-5]
$C_7H_9NO_2$ 139.154
Reddish-brown needles (toluene). Mp 175-180°. Blackens at 160°. Aq. solns. discolour in air.

3-Me ether, N*-Ac: 4-Hydroxy-2-methoxyacetanilide*
[5307-06-2]
$C_9H_{11}NO_3$ 181.191
Isol. from a fungal endophyte of spruce needles and from a soil fungus. Also prod. by a marine-derived *Penicillium* sp. Red needles (toluene). Mp 169-171°.

Di-Me ether: 2,4-Dimethoxyaniline
[2735-04-8]
$C_8H_{11}NO_2$ 153.18
Alarm pheromone isol. from *Neanura muscorum*. Plates (petrol) or oil. Mp 32.5-33.5°. $Bp_{0.006}$ 75-80°.

▶ LD_{50} (rat, orl) 464 mg/kg. BX4200000

Di-Me ether; hydrochloride: [54150-69-5]
Mp 230° dec.

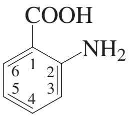
[37966-57-7]

Collins, R.F. *et al., J.C.S.(C)*, 1966, 366 (*synth*)
Messer, C. *et al., CA*, 1999, **131**, 71415y (*2,4-Dimethoxyaniline, isol*)

2-Aminobenzoic acid, 9CI A-706

Anthranilic acid, 8CI. Vitamin L₁

[118-92-3]
[1321-11-5]



$C_7H_7NO_2$ 137.138

Prod. by bacteria and fungi. An important intermed. in the synth. of many compds., corrosion inhibitor for metals. Used as 3% aq. soln. of Na salt for gravimetric detn. of Co, Ni, Cu(*II*), Hg(*II*), Mn, Pb, Cd, U(*VI*), Zn. Inducer of fruiting body formation. Transient receptor potential (TRP) channel blocker. Leaflets. Sol. hot H_2O, EtOH, Et_2O. Mp 144-148°. pK_{a1} 1.97; pK_{a2} 4.79 (25°). pK_{a1} 2.17; pK_{a2} 4.85 (25°, 0.1*M* KCl). Sublimes, triboluminescent. λ_{max} 218 (ϵ 20200); 248 (ϵ 7000); 335 (ϵ 4700) (MeOH) (Berdy).

▶ LD_{50} (mus, orl) 1400 mg/kg. Exp. reprod. effects. CB2450000

Hydrochloride: [2099-63-0]
Mp 193-194°.

β-D-Glucopyranosyl ester: β-D-Glucopyranosyl anthranilate
[55798-72-6]
$C_{13}H_{17}NO_7$ 299.28
Constit. of the fruit of piñuela (*Bromelia plumieri*, Bromeliaceae) and of *Arabidopsis thaliana.*

α-L-Rhamnopyranosyl ester: α-L-Rhamnopyranosyl anthranilate
$C_{13}H_{17}NO_6$ 283.28
Prod. by *Actinomyces* sp. Stamm K 17/2. Amorph. solid. $[\alpha]_D^{20}$ -76 (c, 0.1 in MeOH). λ_{max} 219 (log ϵ 4.25); 249 (log ϵ 3.72); 341 (log ϵ 3.55) (MeOH).

6-Deoxy-α-L-talopyranosyl ester: 2-Aminobenzoyl 6-deoxy-α-L-talopyranoside
$C_{13}H_{17}NO_6$ 283.28
Prod. by *Streptomyces* sp. GöM1. Amorph. solid. λ_{max} 219 (log ϵ 3.93); 248 (log ϵ 3.43); 340 (log ϵ 3.19) (MeOH).

Me ester: Methyl 2-aminobenzoate. FEMA 2682
[134-20-3]
$C_8H_9NO_2$ 151.165
Found in essential oils, including bergamot, orange peel, lemon peel, jasmine, ylang-ylang and neroli. Also present in concord grape, strawberry, star fruit, black tea and rice bran. Found in egg masses of the muricid mollusc *Truncularìopsis trunculus.* Used in perfumery as artificial orange blossom fragrance, also employed extensively in the form of its Schiff's bases (e.g. with Hydroxycitronellal). Flavouring agent. Cryst. Mp 24-25°. Bp_{15} 133.5°. pK_a 2.32 (25°, 1% EtOH aq.). Steam-volatile.

▶ Skin irritant. LD_{50} (rat, orl) 2910 mg/kg. Exp. reprod. effects. CB3325000

Et ester: Ethyl 2-aminobenzoate. FEMA 2421
[87-25-2]
$C_9H_{11}NO_2$ 165.191
Present in orange and grape. Flavouring ingredient. Liq. with faint orange-flower odour and flavour. d_4^{20} 1.12. Mp 13°. Bp 266-268° Bp_{15} 145-147°.

▶ DG2448000

Amide: 2-Aminobenzamide. Anthranilamide
[88-68-6]
$C_7H_8N_2O$ 136.153
Prod. by a marine *Cytophaga marinoflava* sp. AM13.1. Acetaldehyde scavenger for polyethylene beverage bottles. Fluorescent label for polysaccharides etc. Leaflets. Mp 109-111.5° dec.

▶ CU8993000

Amide, N^2*-(2*S*-hydroxypropanoyl): 2-[(2-Hydroxypropanoyl)amino]benzamide*
[18326-27-7]
$C_{10}H_{12}N_2O_3$ 208.216
Prod. by *Penicillium chrysogenum*. Oil.

N*-Eicosanoyl:* N*-Eicosanoylanthranilic acid.* N*-Arachidylanthranilic acid*
[165393-50-0]
$C_{27}H_{45}NO_3$ 431.657
Constit. of *Inula japonica* and *Ononis natrix*. Cryst. (MeOH). Mp 86-87°.

N*-Docosanoyl:* **N-*Docosanoylanthranilic acid***
[85563-88-8]
$C_{29}H_{49}NO_3$ 459.711
Constit. of *Inula oculus-christi* and *Inula japonica*. Cryst. (Me_2CO/petrol). Mp 91-93°.

N*-Docosanoyl, Et ester:* ***Ethyl* N*-docosanoylanthranilate***
[209523-04-6]
$C_{31}H_{53}NO_3$ 487.765
Constit. of the roots of *Gentiana tibetica*. Antifungal agent.

N-*(13Z-Docosenoyl):* N-*(13-Docosenoyl)anthranilic acid*
[129277-41-4]
$C_{29}H_{47}NO_3$ 457.695
Constit. of *Ononis natrix* ssp. *hispanica*. Oil.

N-*Tricosanoyl:* **N-*Tricosanoylanthranilic acid***
$C_{30}H_{51}NO_3$ 473.738
Constit. of *Inula japonica*.

N-*Tetracosanoyl:* **N-*Tetracosanoylanthranilic acid***
$C_{31}H_{53}NO_3$ 487.765
Constit. of *Inula japonica*.

N-*(Carboxyacetyl): 2-[(Carboxyacetyl)amino]benzoic acid, 9CI.* ***2-(Malonylamino)benzoic acid***
[53947-84-5]
$C_{10}H_9NO_5$ 223.185
Isol. from the leaves of the peanut (*Arachis hypogaea*). Cryst. (Me_2CO/hexane). Mp 190-192°.

N-*(3ξ-Hydroxyeicosanoyl):* **N-*(3-Hydroxyeicosanoyl)anthranilic acid***
[856686-30-1]
$C_{27}H_{45}NO_4$ 447.657
Constit. of the aerial parts of *Ononis natrix*.

N-*Succinoyl:* **N-*Succinoylanthranilic acid***
[5694-37-1]
[120572-43-2 (Et ester)]
$C_{11}H_{11}NO_5$ 237.212
Alkaloid from *Aconitum septentrionale*. Cryst. (Me_2CO) (as di-Et ester). Mp 57-58° (di-Et ester). Prob. artifact.

N-*Succinoyl, Me ester:* ***Methyl* N-*succinoylanthranilate***
[108540-96-1]
$C_{12}H_{13}NO_5$ 251.238
Constit. of *Aconitum laeve*. Amorph. powder.

N-*[3-(Methoxycarbonyl)propanoyl], Me ester:* [59868-50-7]
$C_{13}H_{15}NO_5$ 265.265
Constit. of the alga *Jolyna laminarioides*. Chymotrypsin inhibitor. Amorph. powder. Mp 50°. λ_{max} 222 ; 251 ; 307 (MeOH).

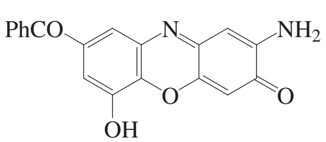
N-*(4-Methylbenzyl): 2-[(4-Methylbenzyl)amino]benzoic acid.* ***Onosmin A***
$C_{15}H_{15}NO_2$ 241.289
Constit. of *Onosma hispida*. Lipoxygenase inhibitor. Amorph. solid. Mp 185-187°. λ_{max} 284 ; 343 (MeOH).

N-*(4-Methylbenzyl), Me ester:* ***Onosmin B***
$C_{16}H_{17}NO_2$ 255.316
Constit. of *Onosma hispida*. Lipoxygenase inhibitor. Amorph. solid. Mp 137-140°. λ_{max} 275 ; 353 (MeOH).

[99196-75-5 , 552-37-4 , 99197-00-9 , 117808-63-6 , 99196-74-4]

Kimura, Y. *et al., Agric. Biol. Chem.*, 1974, **38**, 1507-1510 (*2-Malonylaminobenzoic acid*)
Malakov, P.Y. *et al., Phytochemistry*, 1982, **21**, 2589-2590 (*Docosanoylanthranilic acid*)
Barrero, A.F. *et al., Phytochemistry*, 1990, **29**, 1967-1969 (*Docosenoylanthranilic acid*)
Al-Khalil, S. *et al., J. Nat. Prod.*, 1995, **58**, 760-763 (*Eicosanoylanthranilic acid*)
Usmanova, S.K. *et al., Khim. Prir. Soedin.*, 1996, **32**, 77-81; *Chem. Nat. Compd. (Engl. Transl.)*, 1996, **32**, 62-65 (*N-succinoyl*)
Tan, R.X. *et al., Phytochemistry*, 1998, **47**, 1223-1226 (*Ethyl docosanoylanthranilate*)
Nawasreh, M. *et al., Alexandria J. Pharm. Sci.*, 2004, **18**, 165-170; *CA*, **143**, 93919r (*N-3-Hydroxyeicosanoylanthranilic acid*)
Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)
Ahmad, I. *et al., Chem. Pharm. Bull.*, 2005, **53**, 907-910 (*Onosmins A,B*)
Shaheen, F. *et al., Phytochemistry*, 2005, **66**, 935-940 (*Methyl N-succinoylanthranilate*)
Wang, J. *et al., Plant J.*, 2005, **44**, 606-619 (*biosynth*)
Bitzer, J. *et al., Eur. J. Org. Chem.*, 2006, 3661-3666 (*6-deoxytalopyranosyl ester*)
Qin, J.J. *et al., Chin. Chem. Lett.*, 2008, **19**, 556-558 (*Inula japonica N-acyl derivs*)

2-Amino-8-benzoyl-6-hydroxy-3*H*-phenoxazin-3-one A-707



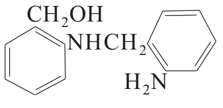
$C_{19}H_{12}N_2O_4$ 332.315
Prod. by marine bacterium *Halomonas* sp. GWS-BW-H8hM. Moderately cytotoxic. Red solid. λ_{max} 257 (log ϵ 3.81); 309 (log ϵ 3.59); 432 (log ϵ 3.46) (MeOH). λ_{max} 254 (log ϵ 3.73); 305 (log ϵ 3.53); 454 (log ϵ 3.57) (MeOH/HCl). λ_{max} 243 (log ϵ 3.89); 438 (log ϵ 3.67) (MeOH/NaOH).

*4′-Hydroxy: 2-Amino-6-hydroxy-8-(4-hydroxybenzoyl)-3*H*-phenoxazin-3-one*
$C_{19}H_{12}N_2O_5$ 348.314
Prod. by *Halomonas* sp. GWS-BW-H8hM. Red solid. λ_{max} 266 (log ϵ 3.54); 300 (log ϵ 3.52); 428 (log ϵ 3.44); 434 (log ϵ 3.45) (MeOH). λ_{max} 249 (log ϵ 3.62); 304 (log ϵ 3.58); 465 (log ϵ 3.35) (MeOH/HCl). λ_{max} 239 (log ϵ 3.61); 346 (log ϵ 3.56); 445 (log ϵ 3.49) (MeOH/NaOH).

Bitzer, J. *et al., J. Antibiot.*, 2006, **59**, 86-92 (*isol, uv, pmr, cmr, ms*)

2-(2-Aminobenzylamino)benzyl alcohol A-708

2-[[(2-Aminophenyl)methyl]amino]benzenemethanol, 9CI
[83326-78-7]

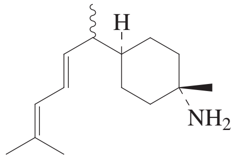


$C_{14}H_{16}N_2O$ 228.293
Isol. from the Indian medicinal plant *Justicia gendarussa* (Acanthaceae). Fine needles ($CHCl_3$/petrol). Mp 131°.

Me ether: ***2-Amino-*N*-[2-(methoxymethyl)phenyl]benzenemethanamine, 9CI***
[83326-77-6]
$C_{15}H_{18}N_2O$ 242.32
From *Justicia gendarussa* (Acanthaceae). Viscous oil.

Chakravarty, A.K. *et al., Tetrahedron*, 1982, **38**, 1797 (*isol*)
Kamat, V.P. *et al., Org. Prep. Proced. Int.*, 1994, **26**, 494 (*synth, pmr*)
Bhattacharyya, S. *et al., Synth. Commun.*, 1995, **25**, 3597 (*synth*)

3-Amino-8,10-bisaboladiene A-709



$C_{15}H_{27}N$ 221.385

(3α,6β,7ξ,8E)-form

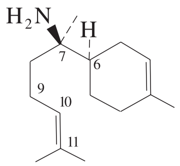
N-*Formyl:* ***3-Formamido-8,10-bisaboladiene***
[134781-22-9]
$C_{16}H_{27}NO$ 249.395
Isol. from the sponge *Halichondria* cf. *lendenfeldi*. Dec. on isol.

Isocyanide: ***3-Isocyano-8,10-bisaboladiene***
[134781-21-8]
$C_{16}H_{25}N$ 231.38
Isol. from the sponge *Halichondria* cf. *lendenfeldi* and the mollusc *Phyllidia pustulosa*. Oil. $[\alpha]_D$ -5.6 (c, 0.2 in $CHCl_3$). Has -NC replacing NH_2. λ_{max} 230 (sh) (ϵ 14000); 237 (ϵ 15300); 246 (sh) (ϵ 11100) (no solvent reported).

Kassühlke, K.E. *et al., J.O.C.*, 1991, **56**, 3747-3750 (*isol, pmr, cmr*)

7-Amino-2,10-bisaboladiene A-710

7-Amino-7,8-dihydro-α-bisabolene. 7-Aminobisabolene



(6R,7R)-form

$C_{15}H_{27}N$ 221.385

(6R,7R)-form [105281-34-3]
Constit. of *Ciocalypta* sp. Oil. $[\alpha]_D$ -15 (c, 0.4 in MeOH).

Hydrochloride: [105281-33-2]
Yellow oil. $[\alpha]_D^{23}$ -8.3 (c, 0.5 in MeOH).

(6R,7S)-form [105281-43-4]
Constit. of a *Halichondria* sp. and a sponge *Theonella* sp. Oil. $[\alpha]_D$ +39 (MeOH). $[\alpha]_D^{20}$ +59.9 (c, 3 in $CHCl_3$).

Δ^9-Isomer, 11-hydroxy: 7-Amino-2,9-bisaboladien-11-ol. ***Aminobisabolenol***
[108384-61-8]
$C_{15}H_{27}NO$ 237.384
Constit. of *Theonella* sp. Oil. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +29 (MeOH).

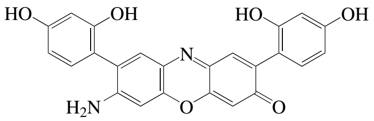
Δ^{11}*-Isomer, 10*R*-hydroxy: 7-Amino-2,11-bisaboladien-10*R*-ol.* ***Isoaminobisabolenol b***
[108384-62-9]
$C_{15}H_{27}NO$ 237.384
Constit. of *Theonella* sp. Oil. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +40 (MeOH).

Δ^{11}*-Isomer, 10*S*-hydroxy: 7-Amino-2,11-bisaboladien-10*S*-ol.* ***Isoaminobisabolenol a***
[108449-15-6]
$C_{15}H_{27}NO$ 237.384
Constit. of *Theonella* sp. Oil. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +34 (MeOH).

Sullivan, B.W. *et al., J.O.C.*, 1986, **51**, 5134-5136 (*Halichondria constits*)
Gulavita, N.K. *et al., J.O.C.*, 1986, **51**, 5136-5139 (*Ciocalypta constit*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1987, **35**, 928 (*Theonella constits, cryst struct*)

7-Amino-2,8-bis(2,4-dihydroxyphenyl)-3*H*-phenoxazin-3-one, 9CI A-711

Resorcein
[33869-21-5]

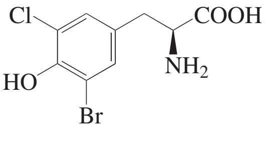


$C_{24}H_{16}N_2O_6$ 428.4
Tentative isolation. Constit. of tobacco leaves. Used in hair preparations and as an elastin stain. Violet needles (C_6H_6/Me_2CO). Dec. at 300°. λ_{max} 587 (MeOH).

Musso, H. *et al., Chem. Ber.*, 1963, **96**, 1579 (*synth, uv*)
Lillie, R.D. *et al., Acta Histochem.*, Suppl., 1971, **No. 9**, 625 (*synth, use*)
Avunddzhyan, E.S. *et al., CA*, 1974, **81**, 166553e (*isol*)

2-Amino-3-(3-bromo-5-chloro-4-hydroxyphenyl)propanoic acid A-712

3-Bromo-5-chlorotyrosine, 9CI. 3-Chloro-5-bromotyrosine (incorr.)



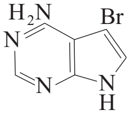
$C_9H_9BrClNO_3$ 294.532

(S)-form
L-form
Isol. from the operculum of *Buccinum undatum* and cuticle of *Limulus polyphemus.*

Hunt, S. *et al., Biochim. Biophys. Acta*, 1971, **252**, 401-404 (*isol*)
Welinder, B.S. *et al., Biochim. Biophys. Acta*, 1972, **279**, 491-497 (*isol, synth, ms*)

4-Amino-5-bromopyrrolo[2,3-*d*]pyrimidine A-713

*5-Bromo-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-amine, 9CI*
[22276-99-9]

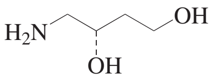


$C_6H_5BrN_4$ 213.036
Isol. from a sponge *Echinodictyum* sp. Bronchodilator and hypotensive agent. Adenosine kinase inhibitor. Needles (EtOH aq.). Mp 240-241° (238-239°) dec. λ_{max} 232 (ϵ 16600); 282 (ϵ 8710) (pH 1) (Derep). λ_{max} 225 (ϵ 14800); 279 (ϵ 8910) (pH 11) (Derep).

Gerster, J.F. *et al., J. Het. Chem.*, 1969, **6**, 207-213 (*synth, uv*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1983, **36**, 165-170 (*isol, uv, pmr, cmr, ms*)

4-Amino-1,3-butanediol A-714

[130239-34-8]



(*S*)*-form*

$C_4H_{11}NO_2$ 105.136

(S)-form [637343-51-2]
Oil.

(±)-form
Oil.

N-E-*Cinnamoyl:* ***Piperlotine K***
[958296-18-9]
$C_{13}H_{17}NO_3$ 235.282
Alkaloid from the leaves of *Piper lolot*. Syrup. Racemate. λ_{max} 211 ; 218 ; 224 ; 280 (MeOH).

N-E-*Cinnamoyl (*E*):* ***Piperlotine J***
[958296-17-8]
$C_{15}H_{19}NO_4$ 277.319
Alkaloid from the leaves of *Piper lolot*. Syrup. Racemate. λ_{max} 212 ; 218 ; 223 ; 280 (MeOH).

(ξ)-form
N-E-*Cinnamoyl, 1,3-di-Ac:* ***Piperlotine L***
[958296-19-0]
$C_{17}H_{21}NO_5$ 319.357
Alkaloid from the leaves of *Piper lolot*. Syrup. $[\alpha]_D$ +42.2 (c, 0.1 in MeOH). λ_{max} 210 ; 216 ; 222 ; 274 (MeOH).

Kuriyama, N. *et al., Synthesis*, 1990, 735-738 (*synth*)
Pat. Coop. Treaty (WIPO), 2003, 03 106 413; *CA*, **140**, 59633 (*S-form, synth*)
Li, C.-Y. *et al., J. Agric. Food Chem.*, 2007, **55**, 9436-9442 (*Piperlotines J,K,L*)

4-Aminobutanoic acid, 9CI A-715

γ-Aminobutyric acid. Piperidinic acid. Piperidic acid. Aminalon. Gamalon. GABA
[56-12-2]
[28805-76-7]

$H_2NCH_2CH_2CH_2COOH$
$C_4H_9NO_2$ 103.121
Widely distributed in higher plants. Prod. by *Monascus pilosus* (Ifo4520). Antihypertensive agent. The natural inhibitory transmitter at synaptic junctions in some regions of the mammalian brain and spinal cord. Prisms (EtOH). V. sol. H_2O; sl. sol. EtOH, Me_2CO; insol. Et_2O. Mp 203° dec. Log P -3.33 (calc). Homopolymers (polyamides) are usually derived from the lactam 2-Pyrrolidinone, P-956.

▶ LD_{50} (mus, orl) 12680 mg/kg. ES6300000

Hydrochloride: Mp 135-136°.

Hydrobromide: [36551-16-3]
Orange solid. Mp 215°.

Me ester: [13031-60-2]
$C_5H_{11}NO_2$ 117.147
Solid (EtOH/Et_2O) (as hydrochloride). Mp 119° (114-115°) (hydrochloride).

▶ ES7065000

Et ester: [5959-36-4]
$C_6H_{13}NO_2$ 131.174
Bp_{12} 75-77°.

Et ester; hydrochloride: Mp 65-72°. Hygroscopic.

▶ LD_{50} (mus, ivn) 425 mg/kg. Exp. reprod. effects.

N-*Ac:* [3025-96-5]
$C_6H_{11}NO_3$ 145.158
Mp 129-131°.

▶ ES5610000

N-*Ac; hydrochloride:* Mp 133°.

N-*(2,2-Dimethylpropanoyl): 4-[(2,2-Dimethyl-1-oxopropyl)amino]butanoic acid, 9CI.* ***Pivagabine, INN***
[69542-93-4]
$C_9H_{17}NO_3$ 187.238
Anticonvulsant.

N-*(5-Hydroxy-3-methyl-2Z-pentenoyl):* ***Fuscoatramide***
$C_{10}H_{17}NO_4$ 215.249
Prod. by *Humicola fuscoatra* NRRL 22980. Oil. λ_{max} 233 (ϵ 3900) (MeOH).

N-tert-*Butyloxycarbonyl:* [57294-38-9]
$C_9H_{17}NO_4$ 203.238
Cryst. (EtOAc/hexane). Mp 53-54°. $Bp_{0.2}$ 78-82°.

N-tert-*Butyloxycarbonyl, anhydride:* [89231-63-0]
$C_{18}H_{32}N_2O_7$ 388.46
Cryst. (EtOAc/petrol). Mp 106°.

N-*Benzyloxycarbonyl:* [5105-78-2]
$C_{12}H_{15}NO_4$ 237.255
Needles (EtOAc/hexane). Mp 65-67°.

N-*Benzyloxycarbonyl, amide:* [35821-20-6]
$C_{12}H_{16}N_2O_3$ 236.27
Cryst. Mp 125-128°.

N-*Me:* [1119-48-8]
$C_5H_{11}NO_2$ 117.147
Cryst. Mp 151.5-153°.

N-*Me; hydrochloride:* [6976-17-6]
Mp 124-126°.

N,N-*Di-Me: 4-(Dimethylamino)butanoic acid*
[693-11-8]
$C_6H_{13}NO_2$ 131.174
Mp 102-104°. Bp_{10} 135-137°.

N,N-*Di-Me; hydrochloride:* Mp 145-147°.

N,N-*Di-Me, Me ester:* [22041-22-1]
$C_7H_{15}NO_2$ 145.201
Sol. H_2O. Mp 171.5-173°.

▶ ES9850000

N-*(2-Nitrobenzenesulfenyl):* [80977-11-3] [104809-33-8]
$C_{10}H_{12}N_2O_4S$ 256.282
Solid. Mp 102° (92.5-94°).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 577C; 577D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 877C (*nmr*)
Org. Synth., Coll. Vol., 2, 1943, 25 (*synth*)
Synge, R.L.M. *et al., Biochem. J.*, 1951, **48**, 429 (*isol*)
Thompson, J.F. *et al., Arch. Biochem. Biophys.*, 1953, **46**, 248 (*synth*)
Reppe, W. *et al., Annalen*, 1955, **596**, 158 (*derivs*)
Goerdler, J. *et al., Angew. Chem.*, 1959, **71**, 775 (*N-(2-nitrophenylsulfenyl), synth*)
Evans, R.L. *et al., J.O.C.*, 1959, **24**, 863-864 (*benzyloxycarbonyl*)
Taddei, F. *et al., J.C.S.*, 1964, 1553 (*pmr*)
Voellmin, J. *et al., Microchem. J.*, 1966, **11**, 73 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 2427 (*occur*)
Steward, E.G. *et al., Acta Cryst. B*, 1973, **29**, 2038; 2825 (*cryst struct*)
Tomita, K. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 2199 (*cryst struct*)
Galzigna, L. *et al., Arch. Int. Pharmacodyn. Ther.*, 1978, **235**, 73 (*Pivagabine*)
Terano, S. *et al., Phytochemistry*, 1978, **17**, 550 (*biosynth*)
Krogsgaard-Larsen, P. *et al., Gaba-Neuro-Transm.: Pharmacochem., Biochem., Pharmacol. Aspects, 1979*, Academic Press, N.Y., 1979,
Rauls, D.O. *et al., J. Med. Chem.*, 1979, **22**, 81-86 (*benzyloxycarbonyl amide*)
Stewart, F.H.C. *et al., Aust. J. Chem.*, 1981, **34**, 2439-2447 (*N-(2-nitrophenylsulfenyl), synth*)
Meldrum, B. *et al., Clin. Neuropharmacol.*, 1982, **5**, 293
Battersby, A.R. *et al., J.C.S. Perkin 1*, 1982, 455 (*biosynth*)
Weber, H.P. *et al., Acta Cryst. B*, 1983, **39**, 360 (*cryst struct*)
Shashua, V.E. *et al., J. Med. Chem.*, 1984, **27**, 659-664 (*tert-butyloxycarbonyl anhydride*)
Blankespoor, R.L. *et al., J.O.C.*, 1984, **49**, 4441-4446 (*benzyloxycarbonyl, synth, ir, pmr*)
Galakatos, N.G. *et al., J.O.C.*, 1985, **50**, 1302 (*deriv, synth, pmr*)
De Feudis, F.V. *et al., Drugs of Today (Barcelona)*, 1986, **22**, 563 (*rev*)
Roberts, E. *et al., Recept. Biochem. Methodol.*, 1986, **5**, 1 (*rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 223 (*synonyms*)
Kirk, D.N. *et al., J.C.S. Perkin 1*, 1988, 2979-2982 (*tert-butyloxycarbonyl*)
Houssin, R. *et al., Synthesis*, 1988, 259-261 (*tert-butyloxycarbonyl*)
Nisticò, G. *et al., GABA: Basic Research and Clinical Applications*, Pythagora Press, 1989, (*book*)
Ramek, M. *et al., Int. J. Quantum Chem.*, 1990, **17**, 45 (*conformn*)
Erdoe, S.L. *et al., J. Neurochem.*, 1990, **54**, 363 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1336
Bon, E. *et al., J.O.C.*, 1994, **59**, 1904 (*synth, ir, pmr, cmr*)
Joshi, B.K. *et al., J. Nat. Prod.*, 2002, **65**, 1734-1737 (*Fuscoatramide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAJ350; PIM500

4-Amino-1-butanol A-716

[13325-10-5]
$H_2NCH_2CH_2CH_2CH_2OH$
$C_4H_{11}NO$ 89.137
Oil. Sol. EtOH, insol. Et_2O. Bp 206° Bp$_{34}$ 125°. Forms a hydrate in water. Absorbs CO_2 and H_2O from air.

▶ LD_{50} (rat, orl) 1150 mg/kg. EK9700000

Picrate: Mp 86.6-88.6°.

N-*Benzyloxycarbonyl:* [17996-13-3]
$C_{12}H_{17}NO_3$ 223.271
Cryst. (EtOAc/hexane). Mp 78-79°.

N-*[3-(Methylthio)-2*E*-propenoyl]:* N-*(4-Hydroxybutyl)-3-(methylthio)-2-propenamide.* ***Aglatenol***
$C_8H_{15}NO_2S$ 189.278
Alkaloid from the leaves of *Aglaia tenuicaulis.* λ_{max} 224 (log ϵ 3.78); 274 (log ϵ 4.32) (MeOH aq.).

N-O-*Bis[3-(methylthio)-2*E*-propenoyl]:* ***Aglatenin***
$C_{12}H_{19}NO_3S_2$ 289.419
Alkaloid from the leaves of *Aglaia tenuiformis.* Cryst. Mp 81-83°. λ_{max} 224 (log ϵ 3.75); 274 (log ϵ 4.49) (MeOH aq.).

N-E-*Cinnamoyl,* O-*[3-(methylthio)-2*E*-propenoyl]:* ***Tenuicaulin A***
$C_{17}H_{21}NO_3S$ 319.424
Alkaloid from the leaves of *Aglaia tenuicaulis.* Cryst. Mp 75-77°. λ_{max} 216 (log ϵ 4.18); 221 (sh) (log ϵ 4.12); 276 (log ϵ 4.52) (MeOH aq.).

N-E-*Cinnamoyl,* O-*[3-(methylthio)-2*Z*-propenoyl]:* ***Isotenuicaulin A***
$C_{17}H_{21}NO_3S$ 319.424
Alkaloid from the leaves of *Aglaia tenuicaulis.* Isol. as a mixt. with Tenucaulin B. λ_{max} 216 (log ϵ 4.17); 221 (sh) (log ϵ 4.12); 282 (log ϵ 4.48) (MeOH aq.).

N-E-*Cinnamoyl,* O-*benzoyl:* ***Caulitenin***
$C_{20}H_{21}NO_3$ 323.391
Alkaloid from the stem bark of *Aglaia tenuicaulis.* λ_{max} 218 (sh) (log ϵ 4.32); 222 (log ϵ 4.32); 231 (sh) (log ϵ 4.18); 274 (log ϵ 4.35) (MeOH aq.).

N,O-*Di*-E-*cinnamoyl:* ***Tenaglin***
$C_{22}H_{23}NO_3$ 349.429
Alkaloid from the stem bark of *Aglaia tenuicaulis.* λ_{max} 216 (log ϵ 4.4); 221 (sh) (log ϵ 4.35); 274 (log ϵ 4.54) (MeOH aq.).

N-Z-*Cinnamoyl,* O-*[3-(methylthio)-2*E*-propenoyl]:* ***Tenucaulin B***
$C_{17}H_{21}NO_3S$ 319.424
Alkaloid from the leaves of *Aglaia tenuicaulis.* Isol. as a mixt. with Isotenucaulin A. λ_{max} 274 (log ϵ 4.16) (MeOH aq.).

N-*Me:* [42042-68-2]
$C_5H_{13}NO$ 103.164
Liq. Bp$_{0.36}$ 71°.

N,N-*Di-Me: 4-(Dimethylamino)-1-butanol, 9CI*
[13330-96-6]
$C_6H_{15}NO$ 117.191
Oil. Bp 186-189° Bp$_{14}$ 80-81°.

Me ether: 4-Methoxy-1-butylamine. 1-Amino-4-methoxybutane
[34039-36-6]
$C_5H_{13}NO$ 103.164
Sol. H_2O, EtOH, Et_2O. Bp 142-145°.

N,N-*Dibutyl:* [94473-23-1]
$C_{12}H_{27}NO$ 201.351
Bp$_{40}$ 172-175°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 338D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 538A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 429A (*ir*)
Henry, L. *et al., Ber.*, 1900, **33**, 3170 (*synth*)
Lunsford, C.D. *et al., J.O.C.*, 1957, **22**, 1225 (*N,N-dibutyl*)
Kaluszyner, A. *et al., J.O.C.*, 1961, **26**, 3536 (*deriv*)
Hoffman, R.V. *et al., J.C.S. Perkin 1*, 1989, 1375 (*deriv*)
Zoppetti, G. *et al., Biochim. Biophys. Acta*, 1992, **1156**, 92 (*N,N-dibutyl*)
Wilk, A. *et al., J.O.C.*, 1999, **64**, 7515-7522 (*N-Me, synth, pmr, cmr*)
Wakayima, T. *et al., Bull. Chem. Soc. Jpn.*, 2004, **77**, 331-340 (*N-benzyloxycarbonyl*)
Greger, H. *et al., Phytochemistry*, 2008, **69**, 928-938 (*Aglaia tenuicaulis alkaloids*)

4-Amino-2-butenoic acid, 9CI A-717

4-Aminocrotonic acid
[25747-40-4]
$H_2NCH_2CH{=}CHCOOH$
$C_4H_7NO_2$ 101.105

(E)-form [38090-53-8] Neurochemical transmission inhibitor. Prisms (EtOH). Sol. H_2O. Mp 164° dec.

(ξ)-form

N-*Ac: 4-(Acetylamino)-2-butenoic acid, 9CI*
[64120-63-4]
$C_6H_9NO_3$ 143.142
Metab. of *Fusarium graminearum.* Cryst. (MeOH/$CHCl_3$). Mp 140°.

Balenovic, K. *et al., J.O.C.*, 1954, **19**, 1589 (*synth*)
Jones, G.P. *et al., J.C.S. Perkin 2*, 1975, 1059 (*cryst struct*)
Vesonder, R.F. *et al., Phytochemistry*, 1977, **16**, 1296 (*deriv, isol*)
Allan, R.D. *et al., Aust. J. Chem.*, 1978, **31**, 2283 (*synth*)

N-(4-Aminobutyl)-*N*-(3-aminopropyl)-1,4-butanediamine, 9CI A-718

5-(3-Aminopropyl)-1,9-diamino-5-azanonane. N^5*-(3-Aminopropyl)homospermidine*
[143085-75-0]
$(H_2NCH_2CH_2CH_2CH_2)_2NCH_2CH_2CH_2NH_2$
$C_{11}H_{28}N_4$ 216.369
Isol. from thermophilic bacteria.

Hamana, K. *et al., Biochem. J.*, 1992, **284**, 741-747

(4-Aminobutyl)guanidine, 9CI A-719

4-Guanidinobutylamine. 1-Amino-4-guanidinobutane. ***Agmatine***
[306-60-5]
$HN{=}^6C(NH_2)NH(CH_2)_3CH_2NH_2$
$C_5H_{14}N_4$ 130.192
Present in ergot, pollen of *Ambrosia artemisiifolia* (Asteraceae), the sea anemone *Anthopleura japonica* and herring semen (*Clupea* sp.). Occurs in *Stichopus japonicus*, *Halocynthia roretzi*, *Crassostrea gigas* and *Tapes philippinarum*. Metab. intermed. for polyamines. Synth. in mammalian brain. Endogenous neurotransmitter. Inhibits hyperalgesia and tolerance to morphine. NMDA receptor antagonist and nitric oxide synthase inhibitor. Mp 101.5-103°.

Sulfate: [2482-00-0]
Cryst. Mp 229° (224-225°).

N^1-*Ac:* **N^1-*Acetylagmatine***
[3031-89-8]
$C_7H_{16}N_4O$ 172.23
Isol. from *Actinia equina* and *Actinia fragacea*.

N^1-*(3*S*-Methyldecanoyl):* ***Aplysillamide B***
[164301-83-1]
$C_{16}H_{34}N_4O$ 298.471
Alkaloid from *Psammaplysilla purea*. Exhibits modest antimicrobial activity against some fungi and bacteria. Not cytotoxic. Oil. Sol. MeOH. $[\alpha]_D^{21}$ -2.4 (c, 0.1 in MeOH) (natural). $[\alpha]_D^{22}$ -5.1 (c, 1.6 in MeOH) (synthetic).

N^1-*(3-Methyl-2*Z*-decenoyl):* ***Aplysillamide A***
[164301-82-0]
$C_{16}H_{32}N_4O$ 296.455
Alkaloid from the Okinawan marine sponge *Psammaplysilla purea*. Exhibits modest antimicrobial activity against some fungi and bacteria. Cytotoxic against murine lymphoma L1210 and human epidermoid carcinoma KB cells. Oil. Sol. MeOH. λ_{max} 225 (ϵ 10000) (MeOH) (Berdy).

N^1-*(4-Hydroxy-*E*-cinnamoyl):* **N^1-trans-p-*Coumaroylagmatine***
[47096-24-2]
[7295-86-5]
$C_{14}H_{20}N_4O_2$ 276.338
Alkaloid from barley seedlings, *Hordeum bulbosum, Hordeum distichon, Hordeum jubatum, Hordeum murinum* and *Hordeum spontaneum* (Poaceae). Exhibits weak antifungal activity. Sol. H_2O. Mp 215-217° (as picrate). λ_{max} 229 (ϵ 33100); 300 (ϵ 26300) (H_2O) (Berdy).

N^1-*(4-Hydroxy-*Z*-cinnamoyl):* **N^1-cis-p-*Coumaroylagmatine***
[191330-81-1]
$C_{14}H_{20}N_4O_2$ 276.338
Constit. of *Albizzia julibrissin*. Leaf-opening factor. Syrup or powder. λ_{max} 278 (ϵ 2000) (H_2O).

N^1-*(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* **N^1-trans-*Feruloylagmatine***
[188305-06-8]
$C_{15}H_{22}N_4O_3$ 306.364
Isol. from *Corydalis saxicola* and from *Triticum aestivum* (wheat) exposed to low temps. Antifungal agent.

N^1-*(3,4-Dimethoxycinnamoyl):* **N^1-*(3,4-Dimethoxycinnamoyl)agmatine***
[128009-18-7]
[146072-40-4]
$C_{16}H_{24}N_4O_3$ 320.391
Alkaloid from *Verbesina caracasana*.

N^6-*Me:* N-*(4-Aminobutyl)*-N′-*methylguanidine.* **N^6-*Methylagmatine***
[77414-15-4]
$C_6H_{16}N_4$ 144.219
Constit. of *Glycine max* and *Medicago sativa*.

N^6-*(3-Methyl-2-butenyl):* N-*(4-Aminobutyl)*-N′-*prenylguanidine.* **N^6-*(3-Methyl-2-butenyl)agmatine***. N^6-*Prenylagmatine*
[128009-17-6]
$C_{10}H_{22}N_4$ 198.311
Alkaloid from *Verbesina caracasana*. Antihypertensive.

N^6-*(3-Methyl-2-butenyl),* N^1-*(3,4-dimethoxycinnamoyl):* see Caracasanamide, C-107

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 821B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1330A (*nmr*)
Kossel, A. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1910, **66**, 257-261; **68**, 170-171 (*isol, struct, synth*)
Heyl, F.W. *et al., J.A.C.S.*, 1919, **41**, 670-682 (*isol*)
Stoessl, A. *et al., Phytochemistry*, 1965, **4**, 973-976 (*isol, uv, struct, synth, N-coumaroyl*)
Boldt, A. *et al., Phytochemistry*, 1971, **10**, 731-738 (*biosynth*)
Smith, T.A. *et al., Phytochemistry*, 1978, **17**, 1093-1098 (*occur, N-coumaroyl*)
Kowabata, T. *et al., CA*, 1979, **89**, 178349 (*isol*)
Robin, Y. *et al., Oceanis*, 1980, **5**, 575-580; *CA*, **94**, 118125p (*N^1-Acetylagmatine*)
Bird, C.R. *et al., Phytochemistry*, 1981, **20**, 2345-2346 (*biosynth, N-coumaroyl*)
Chandrasekhar, K. *et al., Acta Cryst. B*, 1982, **38**, 2538-2540 (*cryst struct*)
Cho, Y.B. *et al., Anal. Biochem.*, 1987, **160**, 429-433 (*N^6-Methylagmatine*)
Matsuzaki, S. *et al., Phytochemistry*, 1990, **29**, 1313-1315 (*N^6-Methylagmatine*)
Hamana, K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 59-62 (*occur, hplc*)
Mitchinson, A. *et al., Chem. Comm.*, 1994, 2613-2614 (*synth*)
Honma, K. *et al., Tetrahedron*, 1995, **51**, 3745 (*Aplysillamides*)
Ueda, M. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2133-2137 (*Z-coumaroyl*)
Reis, D.J. *et al., Ann. N.Y. Acad. Sci.*, 1999, **881**, 65-80 (*rev, activity*)
Monache, G.D. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 3249-3254 (*Prenylagmatine, Dimethoxycinnamoylagmatine*)
Jin, S. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1614-1617 (*Feruloylagmatine*)
Fairbanks, C.A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2000, **97**, 10584-10589 (*pharmacol*)
Reis, D.J. *et al., Trends Pharmacol. Sci.*, 2000, **21**, 187-193 (*pharmacol, rev*)
Demady, D.R. *et al., Mol. Pharmacol.*, 2001, **59**, 24-29 (*pharmacol*)
Cheng, X. *et al., Chem. Biodiversity*, 2008, **5**, 1335-1344 (*Feruloylagmatine*)

(4-Aminobutyl)urea, 8CI A-720

N-***Carbamoylputrescine***
[6851-51-0]
$H_2NCH_2(CH_2)_3NHCONH_2$
$C_5H_{13}N_3O$ 131.177
Alkaloid from *Hordeum vulgare* (barley) and *Sesamum indicum* (sesame) (K-deficient plants)(Poaceae, Pedaliaceae).

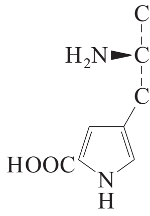
Hydrochloride: Mp 185-186°.

Dipicrate: Mp 164-165°.

Linneweh, F. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1932, **205**, 126; *CA*, **26**, 3276 (*synth*)
Smith, T.A. *et al., Phytochemistry*, 1964, **3**, 23 (*occur, synth*)
Crocomo, O.J. *et al., Phytochemistry*, 1970, **9**, 1487 (*occur*)

4-(2-Amino-2-carboxyethyl)-1*H*-pyrrole-2-carboxylic acid A-721

3-(2-Carboxy-4-pyrrolyl)alanine. 2-Amino-3-(2-carboxy-4-pyrrolyl)propanoic acid



$C_8H_{10}N_2O_4$ 198.178

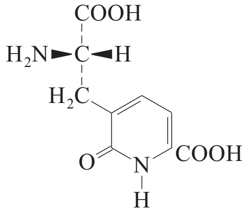
(S)-form
L-form
[137309-97-8]
Isol. from the toxic mushroom *Clitocybe acromelalga*. Mp 200-202° dec.

(±)-form
Mp 200-202° dec.

Yamano, K. *et al., Tetrahedron*, 1992, **48**, 1457 (*isol, synth, struct*)

α-Amino-6-carboxy-2-oxo-3-pyridinepropanoic acid A-722

3-(6-Carboxy-2-oxo-4-pyridinyl)alanine

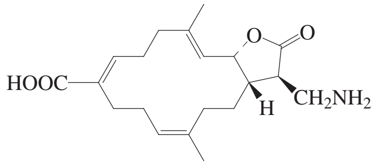


$C_9H_{10}N_2O_5$ 226.188
Sol. H_2O, MeOH; poorly sol. EtOAc, hexane. λ_{max} 241 (ϵ 12000); 315 (ϵ 13500) (H_2O) (Berdy).

(S)-form [148001-20-1]
Isol. from the toxic mushroom *Clitocybe acromelalga*. $[\alpha]_D^{23}$ -5.8 (c, 0.13 in H_2O).

Yamano, K. *et al., Heterocycles*, 1993, **35**, 125 (*isol, struct*)
Yamano, K. *et al., Tetrahedron*, 1993, **49**, 2427 (*isol*)

17-Amino-3,7,11-cembratrien-16,2-olid-19-oic acid A-723



$C_{20}H_{29}NO_4$ 347.453

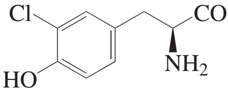
(1*S*,2*S*,3*E*,7*E*,11*E*,15*R*)-*form*

N,N-*Di-Me: 17-Dimethylaminolobohedleolide (incorr.)*
[267007-12-5]
$C_{22}H_{33}NO_4$ 375.507
Constit. of a *Lobophytum* sp.
Shows moderate anti-HIV activity.
Gum. $[\alpha]_D$ +13.1 (c, 0.25 in $CHCl_3$).
λ_{max} 218 (log ϵ 3.6); 222 (log ϵ 3.56) (EtOH).

Rashid, M.A. *et al., J. Nat. Prod.*, 2000, **63**, 531-533 (*isol, pmr, cmr*)

2-Amino-3-(3-chloro-4-hydroxyphenyl)propanoic acid A-724

3-Chlorotyrosine. Monochlorotyrosine
[7298-90-0]



(*S*)-*form*

$C_9H_{10}ClNO_3$ 215.636

(*R*)-*form*

D-form
[162599-96-4]
[905309-56-0 (hydrochloride)]
Mp 255-256° dec. $[\alpha]_D^{20}$ +26 (c, 0.9 in H_2O). $[\alpha]_D$ -12 (c, 3.05 in MeOH).

N-*(3-Methoxycarbonyl-2*E*-propenoyl): **Xylariamide A***
[853259-88-8]
$C_{14}H_{14}ClNO_6$ 327.72
Isol. from *Xylaria* sp. (FRR 5657).
Pale yellow gum. $[\alpha]_D^{24}$ -22 (c, 0.06 in MeOH). λ_{max} 202 (log ϵ 4.05); 217 (sh) (log ϵ 3.74); 278 (log ϵ 3.12) (MeOH).

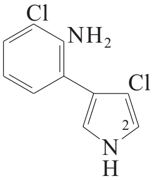
(*S*)-*form*

L-form
[7423-93-0]
Isol. from hydrolysates of mollusc (*Buccinum undatum*) scleroproteins and insect cuticle (*Schistocerca gregaria* and *Limulus polyphemus*). $[\alpha]_D^{20}$ -26.2.

Dibbo, A. *et al., J.C.S.*, 1961, 2645-2651 (*R-form, synth*)
Welinder, B.S. *et al., Biochim. Biophys. Acta*, 1972, **279**, 491-497 (*isol, ms*)
Hunt, S. *et al., FEBS Lett.*, 1972, **24**, 109-112 (*isol*)
Patel, V.F. *et al., J. Med. Chem.*, 1999, **42**, 2588-2603 (*synth, pmr, cmr*)
Davis, R.A. *et al., J. Nat. Prod.*, 2005, **68**, 769-772 (*Xylariamide A*)
Davis, R.A. *et al., Tet. Lett.*, 2005, **46**, 5199-5201 (*Xylariamide A, synth*)

3-(2-Amino-3-chlorophenyl)-4-chloro-1*H*-pyrrole, 8CI A-725

*2-Chloro-6-(4-chloro-1*H*-pyrrol-3-yl)benzenamine, 9CI. **Aminopyrrolnitrin**. WB 2838. Antibiotic WB 2838*
[16386-65-5]



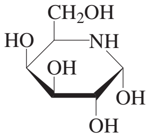
$C_{10}H_8Cl_2N_2$ 227.092
Prod. by *Pseudomonas aureofaciens* and *Pseudomonas cepacia*. Androgen-receptor antagonist and antifungal agent. Pale yellow needles (MeOH aq.). Mp 91° (synthetic). Similar to Pyrrolnitrin, P-961. λ_{max} 216 (ϵ 21400); 270 (ϵ); 299 (ϵ 3890) (solvent not reported) (Derep).

*2-Chloro: **4-(2-Amino-3-chlorophenyl)-2,3-dichloro-1*H*-pyrrole**. Aminochloropyrrolnitrin*
[124201-43-0]
$C_{10}H_7Cl_3N_2$ 261.537
From *Pseudomonas cepacia*. λ_{max} 212 (ϵ 34500); 302 (ϵ 4080) (MeOH) (Berdy).

Salcher, O. *et al., Tet. Lett.*, 1978, 3097 (*isol, pmr*)
Roitman, J.N. *et al., Appl. Microbiol. Biotechnol.*, 1990, **34**, 381 (*isol*)
Roitman, J.N. *et al., J. Agric. Food Chem.*, 1990, **38**, 538 (*isol*)
Hori, Y. *et al., J. Antibiot.*, 1993, **46**, 1327 (*isol, props*)

5-Amino-5-deoxygalactose A-726

*6-Hydroxymethyl-2,3,4,5-piperidinetetrol, 9CI. **Galactostatin**.* galacto-*Nojirimycin. 5-Amino-5-deoxygalactopyranose*



α-D-Pyranose-*form*

$C_6H_{13}NO_5$ 179.172
Log P -3.55 (calc).

D-*form* [107537-94-0]
Isol. from *Streptomyces lydicus*
. β-Galactosidase inhibitor. Amorph. solid + ½ H_2O or syrup. Mp 94-98°. $[\alpha]_D^{23}$ +85.6 (c, 1 in H_2O). Stable up to 5d at 4°.

Bisulfite adduct: Mp 149-150°. $[\alpha]_D$ +19 (c, 0.8 in H_2O).

D-Pyranose-*form*

Pentakis(trimethylsilyl): [40222-80-8]
$C_{21}H_{53}NO_5Si_5$ 540.081
Liq.

α-D-Furanose-*form*

*1,2-Isopropylidene: 5-Amino-5-deoxy-1,2-*O*-isopropylidene-α-D-galactofuranose*
$C_9H_{17}NO_5$ 219.237
Hygroscopic solid. $[\alpha]_D^{22}$ -25.3 (c, 1.0 in MeOH).

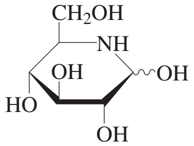
*6-Trityl, 1,2-isopropylidene: 5-Amino-5-deoxy-1,2-*O*-isopropylidene-6-*O*-trityl-α-D-galactofuranose*
$C_{28}H_{31}NO_5$ 461.557
Mp 135°. $[\alpha]_D^{23}$ -11.5 (c, 1.0 in $CHCl_3$).

[40222-81-9 , 108147-56-4 , 109718-63-0]

Inouye, S. *et al., CA*, 1973, **78**, 47847g (*silyl deriv*)
Legler, G. *et al., Carbohydr. Res.*, 1986, **155**, 119 (*α-D-fur deriv*)
Miyake, Y. *et al., J. Antibiot.*, 1987, **40**, 122-123 (*isol*)
Miyake, Y. *et al., Agric. Biol. Chem.*, 1988, **52**, 153-158; 661-666 (*isol, pmr, cmr, struct, props*)
Aoyagi, S. *et al., J.O.C.*, 1991, **56**, 815-819 (*synth*)
Chida, N. *et al., Chem. Comm.*, 1994, 1247-1248 (*synth*)
Kirihata, M. *et al., Heterocycles*, 1995, **41**, 2271 (*synth*)
Dondoni, A. *et al., J.O.C.*, 1995, **60**, 4749 (*synth, pmr*)
Pérez, P.D. *et al., Eur. J. Org. Chem.*, 2005, 2903-2913 (*α-D-fur 1,2-isopropylidene*)

5-Amino-5-deoxyglucose, 9CI, 8CI A-727

6-(Hydroxymethyl)-2,3,4,5-piperidinetetrol



D-Pyranose-*form*

$C_6H_{13}NO_5$ 179.172

D-Pyranose-*form*

Nojirimycin
[15218-38-9]
[19130-94-0 (α-D-pyr-form)]

Amino sugar antibiotic. Produced by several *Streptomyces* spp. Primarily active against gram-positive bacteria. Sol. H_2O; fairly sol. MeOH, EtOH; poorly sol. butanol, hexane. Mp 126-130° dec. $[\alpha]_D^{24}$ +100 (3 min.) → +73.5 (20 hr.).

▸ LD_{50} (mus, ipr) 1600 mg/kg; LD_{50} (mus, ivn) 1250 mg/kg. LZ5655000

1-Deoxy: see 2-(Hydroxymethyl)-3,4,5-piperidinetriol, H-616

L-Pyranose-*form*

Mp 122-124°. $[\alpha]_D^{20}$ -72.1 (c, 0.3 in H_2O).

α-D-Furanose-*form*

*1,2-*O*-Isopropylidene: 5-Amino-5-deoxy-1,2-*O*-isopropylidene-α-D-glucofuranose*
[16958-27-3]
$C_9H_{17}NO_5$ 219.237
Cryst. (EtOAc). Mp 125-126° Mp 175°. $[\alpha]_D^{25}$ -13.75 (c, 4 in MeOH). Higher Mp product (2004) may be the β-L-*ido*-analogue.

*1,2:3,6-Diisopropylidene: 5-Amino-5-deoxy-1,2:3,6-di-*O*-isopropylidene-α-D-glucofuranose*

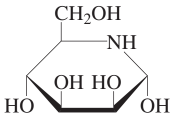
$C_{12}H_{21}NO_5$ 259.302
Needles (EtOAc/heptane). Mp 68-69°.

1,2-O-Isopropylidene, N-3,6-tri-Ac: 5-Acetamido-3,5-di-O-acetyl-5-deoxy-1,2-O-isopropylidene-α-D-glucofuranose
[16958-28-4]
$C_{15}H_{23}NO_8$ 345.349
Needles (Et_2O). Mp 145-146°. $[\alpha]_D^{25}$ +1.3 (c, 6 in $CHCl_3$).

Inouye, S. *et al., J. Antibiot.*, 1966, **19**, 288 (*struct, nmr*)
Saeki, H. *et al., Chem. Pharm. Bull.*, 1968, **16**, 962 (*synth*)
Nayak, U.G. *et al., J.O.C.*, 1968, **33**, 3582-3585 (*α-D-fur isopropylidene, α-D-fur isopropylidene tri-Ac*)
Inouye, S. *et al., Tetrahedron*, 1968, **24**, 2125 (*ir, ms, nmr, struct, synth*)
Ger. Pat., 1978, 2 658 561; *CA*, **89**, 152713 (*use*)
Kinast, G. *et al., Angew. Chem., Int. Ed.*, 1981, **20**, 805 (*bibl*)
Austrian Pat., 1982, 366 032; *CA*, **97**, 90401 (*synth*)
Vasella, A. *et al., Helv. Chim. Acta*, 1982, **65**, 1134 (*synth*)
Ezure, Y. *et al., Agric. Biol. Chem.*, 1985, **49**, 1119 (*isol, bibl*)
Iida, H. *et al., J.O.C.*, 1987, **52**, 3337 (*synth*)
Tsuda, Y. *et al., Heterocycles*, 1988, **27**, 63 (*synth*)
Kayakiri, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1397-1401 (*α-D-fur isopropylidene*)
Chida, N. *et al., Carbohydr. Res.*, 1992, **237**, 185 (*synth*)
Dondoni, A. *et al., Tetrahedron*, 1993, **49**, 2939 (*synth, L-form*)
Dondoni, A. *et al., Chem. Eur. J.*, 1995, **1**, 505-520 (*α-D-fur isopropylidene*)
Moutel, S. *et al., J.C.S. Perkin 1*, 1999, 1403-1406 (*synth*)
Gottschaldt, M. *et al., Carbohydr. Res.*, 2004, **339**, 1941-1952 (*α-D-fur isopropylidene, α-D-fur diisopropylidene*)
Morwenna, M.S.M. *et al., Eur. J. Org. Chem.*, 2005, 2159-2191 (*rev, synth*)

5-Amino-5-deoxymannose A-728

Nojirimycin B. *Mannonojirimycin. Mannojirimycin*



α-D-Pyranose-*form*

$C_6H_{13}NO_5$ 179.172
Aminoglycoside antibiotic.

D-Pyranose-*form* [62362-40-7]
Prod. by *Streptomyces lavendulae* SF-425. Weakly active against *Xanthomonas oryzae*. Glucosidase and mannosidase inhibitor. Pale yellow powder. Sol. H_2O; poorly sol. Me_2CO, hexane. Unstable.

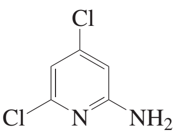
Bisulfite adduct:
Needles (H_2O). Mp 163-165° dec. $[\alpha]_D^{20}$ +4.6 (c, 0.5 in H_2O).

L-Pyranose-*form*
Mp 162-164° (as bisulfite adduct). $[\alpha]_D^{20}$ -4.5 (c, 0.31 in H_2O).

Japan. Pat., 1976, 76 151 393; *CA*, **86**, 153954 (*isol*)
Niwa, T. *et al., J. Antibiot.*, 1984, **37**, 1579 (*isol, cryst struct, props, nmr, ir*)
Dondoni, A. *et al., Tetrahedron*, 1993, **49**, 2939 (*L-form*)

2-Amino-4,6-dichloropyridine A-729

4,6-Dichloro-2-pyridinamine



$C_5H_4Cl_2N_2$ 163.005
Reported from Ku Shu (*Picrasma quassioides*). Cryst. (petrol). Mp 112.5°.

N-Ac: [63763-91-7]
$C_7H_6Cl_2N_2O$ 205.043
Cryst. (EtOH). Mp 218-219°.

2-N,N-Di-Me: 4,6-Dichloro-N,N-dimethyl-2-pyridinamine, 9CI. 2,4-Dichloro-6-(dimethylamino)pyridine
[849937-99-1]
$C_7H_8Cl_2N_2$ 191.059
Platelets (hexane). Mp 45-46°.

Den Hertog, H.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1950, **69**, 673-699 (*synth*)
Li, T.S.C. *et al., Chinese and Related North American Herbs*, CRC Press, 2002, 113 (*occur*)
Schlosser, M. *et al., J.O.C.*, 2005, **70**, 2494-2502 (*di-Me*)

4-Amino-1,13-diguanidino-5-tridecanone A-730

$HN{=}C(NH_2)NH(CH_2)_8CO^4CH(NH_2)CH_2CH_2CH_2NHC(NH_2){=}NH$

$C_{15}H_{33}N_7O$ 327.472

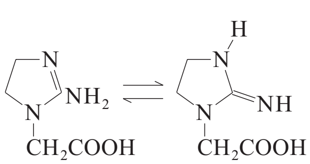
N^4*-Ac:* [167103-52-8]
$C_{17}H_{35}N_7O_2$ 369.509
Isol. from the fermentation broth of an actinomycete (SCC 2268) prob. belonging to the genus *Streptomyces.* Muscarinic receptor antagonist. Sol. H_2O, MeOH; poorly sol. EtOAc, hexane. Mp 250°.

N^4*-(9-Guanidinononanoyl):*
$C_{25}H_{52}N_{10}O_2$ 524.752
Isol. from SCC 2268 broth. Muscarinic receptor antagonist. Sol. H_2O, MeOH; poorly sol. EtOAc, hexane. Mp 250°. $[\alpha]_D^{26}$ -30 (c, 0.3 in H_2O).

Hegde, V.R. *et al., J. Nat. Prod.*, 1995, **58**, 843 (*isol, ir, pmr, cmr, struct*)

2-Amino-4,5-dihydro-1*H*-imidazole-1-acetic acid, 9CI A-731

2-Imino-1-imidazolidineacetic acid. 1-(Carboxymethyl)-2-iminoimidazolidine. Cyclocreatine
[35404-50-3]



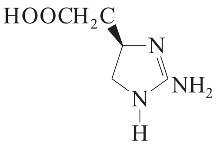
$C_5H_9N_3O_2$ 143.145
Substrate for creatine kinase *in vitro.*

3-Phosphate: 1-(Carboxymethyl)-2-imino-3-phosphonoimidazolidine
[61839-19-8]
$C_5H_{10}N_3O_5P$ 223.125
Source of high energy phosphate. Stored in muscle, heart and brain.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1329B (*nmr*)
Struve, G.E. *et al., J.O.C.*, 1977, **42**, 4035 (*synth, cmr, struct*)
Woznicki, D.T. *et al., J. Neurochem.*, 1979, **33**, 75 (*formn*)
Phillips, G.N. *et al., J.A.C.S.*, 1979, **101**, 7120 (*bibl, cryst struct, phosphate*)
Roberts, J.J. *et al., Arch. Biochem. Biophys.*, 1983, **220**, 563 (*activity*)

2-Amino-4,5-dihydro-1*H*-imidazole-4-acetic acid, 9CI A-732

2-[2-Amino-2-imidazolin-4-yl]acetic acid
[69098-41-5]



(*R*)−*form*

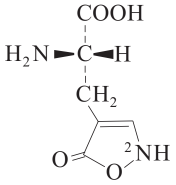
$C_5H_9N_3O_2$ 143.145

(*R*)-*form* [65388-06-9]
Isol. from the seeds of *Lonchocarpus* spp. Cryst. (EtOH/Et_2O).

Fellows, L.E. *et al., Phytochemistry*, 1977, **16**, 1957 (*isol, ir, pmr, cmr, ms, struct*)
Evans, S.V. *et al., Biochem. Syst. Ecol.*, 1985, **13**, 271 (*isol*)

α-Amino-2,5-dihydro-5-oxo-4-isoxazolepropanoic acid, 9CI A-733

α-Amino-5-oxo-3-isoxazoline-4-propionic acid, 8CI. 3-(Isoxazolin-5-on-4-yl)alanine. 4-Alanyl-3-isovalin-5-one. TAN 950A. Antibiotic TAN 950A



$C_6H_8N_2O_4$ 172.14
Exists in tautomeric equilibrium with Antibiotic TAN 950B. λ_{max} 253 (ϵ 8060) (H_2O) (Derep).

(*S*)-*form*
L-form
[127607-88-9]
Prod. by *Streptomyces platensis.* Antifungal agent. Powder + $1H_2O$ (as Na salt). Sol. H_2O, DMSO, DMF; poorly sol. Me_2CO, $CHCl_3$, EtOAc. $[\alpha]_D^{23}$ -69.5 (c, 0.52 in H_2O) (as Na salt). λ_{max} 253 (E1%/1cm 380) (H_2O) (Berdy). λ_{max} 259 (E1%/1cm 421) (HCl) (Berdy).

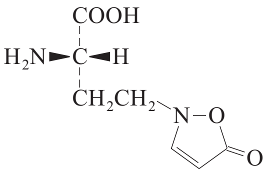
N^2*-β-D-Glucosyl:* [29790-46-3]
$C_{12}H_{18}N_2O_9$ 334.282
Isol. from *Pisum sativum* and *Lathyrus odoratus.* Cryst. (MeOH/propanol). Mp 182° dec.

[130620-29-0 , 130621-41-9 , 130621-42-0 , 130621-61-3]

Lambein, F. *et al., Biochem. Biophys. Res. Commun.*, 1970, **40**, 557; 1974, **61**, 155 (*isol, struct, uv, pmr, ir*)
Murakoshi, I. *et al., Phytochemistry*, 1975, **14**, 1515 (*biosynth*)
Iwama, T. *et al., Eur. J. Pharmacol.*, 1991, **197**, 187 (*props*)
Tsubotani, S. *et al., Tetrahedron*, 1991, **47**, 8079-8090 (*synth, cryst struct*)
Hakoda, S. *et al., J. Antibiot.*, 1992, **45**, 854 (*isol*)

2-Amino-4-(2,5-dihydro-5-oxo-2-isoxazolyl)butanoic acid A-734

2-Amino-4-(isoxazolin-5-on-2-yl)butanoic acid
[59476-62-9]

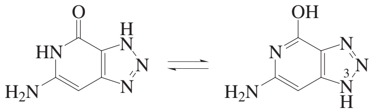


$C_7H_{10}N_2O_4$ 186.167
Incorrect (3-isoxazolyl) struct. in published work. Isol. from sweet pea extracts. Cryst. L-Config. not stated but assumed on biogenetic grounds.

Lambein, F. *et al., Biochem. Biophys. Res. Commun.*, 1974, **61**, 155 (*isol, struct*)
Kuo, Y.H. *et al., Arch. Int. Physiol. Biochim.*, 1976, **84**, 169 (*isol*)
Tamura, N. *et al., Chem. Pharm. Bull.*, (Footnote to), 1992, **40**, 381 (*struct*)

5-Amino-1,6-dihydro-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one, 9CI A-735

8-Azaguanine. Guanazole†*. Pathocidin. NSC 749. SF 337. Antibiotic SF 337. Azan*
[134-58-7]



$C_4H_4N_6O$ 152.115
The name 8-Azaguanine comes from the alternative purine numbering. Systematic (CAS) numbering shown. Isol. from *Streptomyces albus* and *Streptomyces morookaensis.* Purine antagonist. Tumour inhibitor. Active against fungi. Cryst. (H_2O). Mp 305° dec. λ_{max} 250 (ϵ 12500); 270 (sh) (ϵ 9880) (0.1*N* HCl) (Derep). λ_{max} 247 (ϵ 4860); 278 (ϵ 6540) (0.1*N* NaOH) (Derep). λ_{max} 247 (ϵ 9580); 273 (ϵ 6300) (H_2O) (Derep).
▸ Exp. reprod. and teratogenic effects. LD_{50} (mus, orl) 1500 mg/kg. XZ6157000

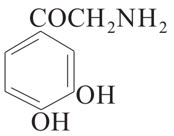
*3*N*-β-*D*-Ribofuranosyl: 8-Azaguanosine*
[2133-80-4]
$C_9H_{12}N_6O_5$ 284.231
Purine antagonist. Mp 250-252° dec. λ_{max} 255 (ϵ 13600); 269 (ϵ 10300) (0.01*N* HCl). λ_{max} 221 (ϵ 23000); 279 (ϵ 11600) (0.03*N* NaOH).
▸ XZ6157200

*3*N*-β-*D*-Ribofuranosyl, 5′-phosphate: 8-Azaguanosine 5′-phosphate*
[1165-66-8]
$C_9H_{13}N_6O_8P$ 364.211
Appears to be the key intermed. in the conversion of the anticancer drug, 8-Azaguanine, into its active form. λ_{max} 256 (ϵ 12900) (pH 2).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 716C (*ir*)
Roblin, R.K. *et al., J.A.C.S.*, 1945, **67**, 290-294 (*synth*)
Friedkin, M. *et al., J. Biol. Chem.*, 1954, **209**, 295-301 (*8-Azaguanosine*)
Davoll, J. *et al., J.C.S.*, 1958, 1593-1599 (*8-Azaguanosine*)
Blank, H.U. *et al., J.O.C.*, 1970, **35**, 1131-1138 (*synth*)
Crit. Rev. Toxicol., 1973, **2**, 159-209 (*tox, rev*)
Kozlowski, D.L. *et al., Acta Cryst. B*, 1975, **31**, 1751-1753 (*cryst struct*)
Elliott, R.D. *et al., J. Med. Chem.*, 1976, **19**, 1186-1191 (*8-Azaguanosine*)
Luedemann, H.D. *et al., Z. Naturforsch., C*, 1976, **31**, 135-140; *CA*, **84**, 146335u (*8-Azaguanosine, conformn, pmr*)
Bose, S.N. *et al., Biomed. Mass Spectrom.*, 1977, **4**, 305-309 (*ms*)
Purnell, L.G. *et al., Org. Magn. Reson.*, 1977, **10**, 1-4 (*cmr*)
Hirasawa, K. *et al., J. Antibiot.*, 1978, **31**, 628-629 (*isol, props*)
Grunberger, D. *et al., Antibiotics (N.Y.)*, 1979, **5**, 110-123 (*rev*)
Contreras, J.G. *et al., Bioorg. Chem.*, 1998, **26**, 345-355 (*tautom*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJO500

2-Amino-3′,4′-dihydroxyacetophenone, 8CI A-736

2-Amino-1-(3,4-dihydroxyphenyl)ethanone. ***Noradrenalone****. Arterenone. 2-Oxodopamine*
[499-61-6]



$C_8H_9NO_3$ 167.164
Isol. from hydrolysates of sclerotized insect cuticle.
▸ AM5900000

N-*Ac:* ***2-Acetamido-3′,4′-dihydroxyacetophenone****.* N-*Acetyl-2-oxodopamine*
$C_{10}H_{11}NO_4$ 209.201
Isol. from the cast-off shells of the cicada, *Cryptotympana* sp. Yellow cryst. Mp 168-175°.

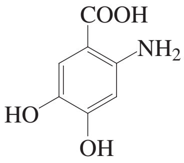
N-*Me: 1-(3,4-Dihydroxyphenyl)-2-(methylamino)ethanone. 3′,4′-Dihydroxy-2-methylaminoacetophenone.* ***Adrenolone, INN, USAN****. Chemosan. Damazor. Haemodan. Kephrine. Ketogaze. Remestyp*†*. Stryphnon. Stypnon. Adrenone*
[99-45-6]
$C_9H_{11}NO_3$ 181.191
Shows similar physiological activity to Adrenaline, A-152. Sympathomimetic, vasoconstrictor and haemostatic agent. Needles. Mp 235-236° dec. Log P 0.32 (calc).
▸ LD_{50} (mus, ivn) 275 mg/kg. AM8050000

N-*Me; hydrochloride:* [62-13-5]
Mp 242°.
▸ AM8225000

Stolz, F. *et al., Ber.*, 1904, **37**, 4152
Friedmann, E. *et al., Chem. Zentralbl.*, 1906, **1**, 1620 (*synth*)
Lands, A.M. *et al., J. Pharmacol. Exp. Ther.*, 1948, **92**, 369 (*pharmacol*)
Ravina, A. *et al., Therapie*, 1953, **8**, 224 (*props, use*)
Remizov, A.L. *et al., Zh. Obshch. Khim.*, 1958, **28**, 2530 (*synth*)
Biniecki, S. *et al., Acta Pol. Pharm.*, 1963, **20**, 245 (*synth*)
Anderson, S.O. *et al., J. Insect Physiol.*, 1970, **16**, 1951 (*isol*)
Bergin, R. *et al., Acta Cryst. B*, 1971, **27**, 2139 (*N-Me, cryst struct*)
Hussain, A. *et al., J. Pharm. Sci.*, 1976, **65**, 1510 (*deriv*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1240
Noda, N. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1749-1752 (*isol, N-Ac*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MGC350

2-Amino-4,5-dihydroxybenzoic acid A-737

6-Aminoprotocatechuic acid. 4,5-Dihydroxyanthranilic acid
[114874-99-6]



$C_7H_7NO_4$ 169.137
Prod. by *Botrytis* sp. AM13791. Inhibitor of protein-tyrosine kinase.

N-*Et, amide: 2-(Ethylamino)-4,5-dihydroxybenzamide, 9CI*
[127793-87-7]
$C_9H_{12}N_2O_3$ 196.205
Alkaloid from *Piper nigrum* (pepper).

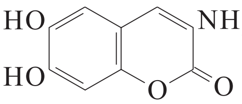
*4-Me ether: 2-Amino-5-hydroxy-4-methoxybenzoic acid. 2-Amino-5-hydroxy-*p*-anisic acid, 8CI*
[31839-21-1]
$C_8H_9NO_4$ 183.163
Mp 214-215° (194-195°).

4-Me ether, N*-(4-hydroxy-3-methoxy-*E*-cinnamoyl):* ***Avenanthramide 2***
[154992-25-3]
$C_{18}H_{17}NO_7$ 359.335
Constit. of *Avena sativa* (oat).

Bandyopadhyay, C. *et al., J. Agric. Food Chem.*, 1990, **38**, 1696-1699 (*N-Et amide*)
Dimberg, L.H. *et al., Cereal Chem.*, 1993, **70**, 637-641 (*Avenanthramide 2*)

3-Amino-6,7-dihydroxy-2*H*-1-benzopyran-2-one, 9CI A-738

3-Amino-6,7-dihydroxycoumarin
[22065-08-3]



$C_9H_7NO_4$ 193.159
Shows hypotensive props. Mp 258-260°.

N-*Formyl: 3-(Formylamino)-6,7-dihydroxycoumarin.* ***Pseudoverdin***
[150624-46-7]
$C_{10}H_7NO_5$ 221.169
Prod. by *Pseudomonas aeruginosa*. Chromophore.

*Di-Me ether: 3-Amino-6,7-dimethoxy-2*H*-1-benzopyran-2-one. 3-Amino-6,7-dimethoxycoumarin*
[150358-93-3]
$C_{11}H_{11}NO_4$ 221.212
Cryst. (EtOH aq.). Mp 170°.

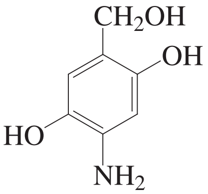
Di-Me ether, N-*formyl:* [150358-91-1]
$C_{12}H_{11}NO_5$ 249.223
Mp 246°.

Di-Me ether, N-*Ac: 3-(Acetylamino)-6,7-dimethoxycoumarin*
[150358-92-2]
$C_{13}H_{13}NO_5$ 263.249
Cryst. (EtOH aq.). Mp 248°.

Fr. Pat., 1968, 1 523 317; *CA*, **72**, 31615v (*synth*)
Longerich, I. *et al., Z. Naturforsch., C*, 1993, **48**, 425 (*isol, synth, derivs*)

4-Amino-2,5-dihydroxybenzyl alcohol A-739

2-Amino-5-(hydroxymethyl)-1,4-benzenediol



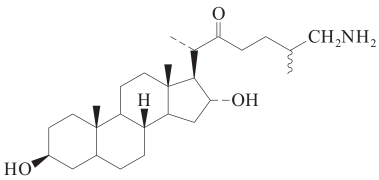
$C_7H_9NO_3$ 155.153

N-*Ac: 2,5-Dihydroxy-4-(hydroxymethyl)acetanilide*
$C_9H_{11}NO_4$ 197.19
Prod. by *Actinomyces* sp. Lu 9419 isol. from *Cetonia aureata*. Solid. Mp 176°. λ_{max} 209 (ϵ 12300); 245 (ϵ 4840); 302 (ϵ 3400) (MeOH).

1′-Me ether, N-*Ac: 2,5-Dihydroxy-4-(methoxymethyl)acetanilide*
$C_{10}H_{13}NO_4$ 211.217
Prod. by *Actinomyces* sp. Lu 9419 isol. from *Cetonia aureata*. Solid.

Schlörke, O. *et al., J. Antibiot.*, 2002, **55**, 635-642 (*N-Ac, isol, pmr, cmr, ms*)

26-Amino-3,16-dihydroxycholestan-22-one A-740



$C_{27}H_{47}NO_3$ 433.673

(3β,5α,16α,25ξ)-*form*

N-*Ac, 3-*O*-[β-D-xylopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Abutiloside B***
[177262-59-8]
$C_{46}H_{77}NO_{17}$ 916.111
Constit. of *Solanum abutiloides*. Solid. $[\alpha]_D^{26}$ -41.9 (c, 0.49 in MeOH).

N-*Butanoyl, 3-*O*-[α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Abutiloside K***
[449178-14-7]
$C_{43}H_{73}NO_{13}$ 812.049
Constit. of *Solanum abutiloides*. Powder. $[\alpha]_D^{25}$ -50.4 (c, 0.25 in MeOH).

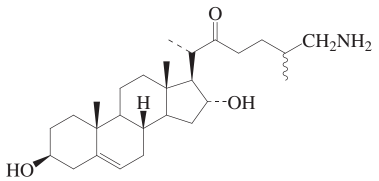
N-*Butanoyl, 3-*O*-[β-D-xylopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Abutiloside J***
[449176-35-6]
$C_{48}H_{81}NO_{17}$ 944.164
Constit. of *Solanum abutiloides*. Powder. $[\alpha]_D^{25}$ -54.1 (c, 0.95 in MeOH).

N-*(3-Methylbutanoyl), 3-*O*-[α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Abutiloside I***
[449176-33-4]
$C_{44}H_{75}NO_{13}$ 826.075
Constit. of *Solanum abutiloides*. Powder. $[\alpha]_D^{25}$ -38.7 (c, 0.15 in MeOH).

N-*(3-Methylbutanoyl), 3-*O*-[β-D-xylopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Abutiloside A***
[171864-79-2]
$C_{49}H_{83}NO_{17}$ 958.191
Constit. of *Solanum abutiloides*. Amorph. powder. $[\alpha]_D^{22}$ -49.2 (MeOH).

Tian, R.-H. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1119-1121 (*isol, pmr, cmr*)
Tian, R.-H. *et al., Phytochemistry*, 1997, **44**, 723-726 (*Abutiloside A*)
Yoshimitsu, H. *et al., Chem. Pharm. Bull.*, 2002, **50**, 284-286 (*Abutilosides I,J,K*)

26-Amino-3,16-dihydroxycholest-5-en-22-one A-741



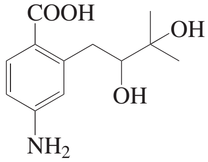
$C_{27}H_{45}NO_3$ 431.657

(3β,16α,26ξ)-*form*

N-*Ac, 3-*O*-[β-D-xylopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Abutiloside H***
[449176-31-2]
Constit. of *Solanum abutiloides*. Powder. $[\alpha]_D^{25}$ -107 (c, 0.2 in MeOH).

Yoshimitsu, H. *et al., Chem. Pharm. Bull.*, 2002, **50**, 284-286

4-Amino-2-(2,3-dihydroxy-3-methylbutyl)benzoic acid A-742



$C_{12}H_{17}NO_4$ 239.271

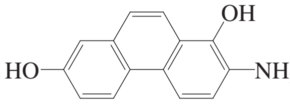
(-)-*form*

Me ester: [1009318-74-4]
$C_{13}H_{19}NO_4$ 253.297
Isol. from *Xylaria* sp. BCC 9653. Gum. $[\alpha]_D^{27}$ -19.2 (c, 0.9 in $CHCl_3$).

Pongcharoen, W. *et al., Chem. Pharm. Bull.*, 2007, **55**, 1647-1648 (*isol, pmr, cmr, ms*)

2-Amino-1,7-dihydroxyphenanthrene A-743

2-Amino-1,7-phenanthrenediol, 9CI



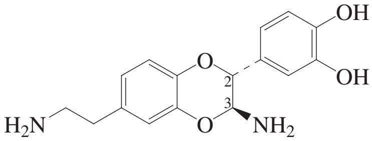
$C_{14}H_{11}NO_2$ 225.246

Di-Me ether, N-*Ac:* N-*(1,7-Dimethoxy-2-phenanthrenyl)acetamide. 2-Acetamido-1,7-dimethoxyphenanthrene*
$C_{18}H_{17}NO_3$ 295.337
Alkaloid from *Sinomenium acutum*. Yellow-green needles. λ_{max} 256 ; 282 ; 310 (no solvent reported).

Cheng, W.M. *et al., Chin. Chem. Lett.*, 2005, **16**, 1481-1483 (*di-Me ether N-Ac, isol, pmr, cmr*)

3-Amino-2-(3,4-dihydroxyphenyl)-2,3-dihydro-1,4-benzodioxin-6-ethanamine A-744

2-Amino-7-(2-aminoethyl)-3-(3,4-dihydroxyphenyl)-1,4-benzodioxan



$C_{16}H_{18}N_2O_4$ 302.329
Dimer of Dopamine, D-920.

(2*R*,3*S*)-*form*

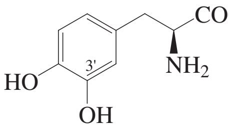
N,N′-*Di-Ac:*

$C_{20}H_{22}N_2O_6$ 386.404
Isol. from the cast-off shells of the cicada *Cryptotympana* sp. Component of Zentai. Yellow powder. Mp 118-126°. $[\alpha]_D$ +51.7 (c, 1 in MeOH).

Noda, N. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1749-1752 (*isol, pmr, cmr*)

2-Amino-3-(3,4-dihydroxyphenyl)propanoic acid A-745

3-Hydroxytyrosine, 9CI. 3,4-Dihydroxyphenylalanine. DOPA
[587-45-1]



(*S*)*-form*

$C_9H_{11}NO_4$ 197.19
Used in treatment of the Parkinsonian syndrome. The immediate precursor of the neurotransmitter dopamine. Usually administered with a peripheral DOPA decarboxylase inhibitor. Intermed. in biosynth. of various marine alkaloids, e.g. the Lamellarins. Log P -2.82 (uncertain value) (calc).

(*R*)*-form*
D-form
[5796-17-8]
Prisms (H_2SO_3 aq.). Mp 282°. $[\alpha]_D$ +11.9.

(*S*)*-form*
L-form. ***Levodopa, BAN, INN, JAN, USAN****. Bendopa. Brocadopa. Dopar. Larodopa. Levopa. Veldopa. Many other names*
[59-92-7]
Occurs in seedlings and pods of *Vicia faba*, in *Mucuna pruriens, Sarothamnus scoparius, Stizolobium deeringianum, Stizolobium hassjoo, Aristolochia clematitis* and other plants. Also prod. by *Bacillus* spp. Prisms, needles ($H_2O + SO_2$) or plates (EtOH aq.). Mp 285.5° dec. $[\alpha]_D^{20}$ -12.15 (c, 4 in 1*N* HCl). Pharmacol. active isomer. Rapidly turns green in air, aq. solns. darken in air. Green col. with $FeCl_3$. Reduces $AgNO_3$, NH_3 and acid $KMnO_4$. Component of Sinemet. High-mol.-wt. polymers have been synth.

▶ Systemic (e.g. CNS) and adverse effects when used therapeutically. LD_{50} (rat, orl) 1780 mg/kg. Exp. reprod. and teratogenic effects. AY5600000

Hydrochloride: [5796-14-5]
Prisms. Mp 209°.

3′-O-Sulfate: 3-(Sulfooxy)tyrosine, 9CI
[96253-55-3]
$C_9H_{11}NO_7S$ 277.254
Constit. of the brown alga *Ascophyllum nodosum.*

3′-O-β-D-Glucopyranoside: [2275-95-8]
$C_{15}H_{21}NO_9$ 359.332
Isol. from *Pisum sativum* (peas) and *Vicia faba*. Resin or syrup.

Me ester: ***Melevodopa, INN****. Levomet*
[7101-51-1]
[1421-65-4]
$C_{10}H_{13}NO_4$ 211.217
Antiparkinsonian agent. Dopamine receptor agonist. Mp 170.5-171.5° (as hydrochloride). $[\alpha]_D^{22}$ +14.7 (c, 12.5 in MeOH) (hydrochloride). CAS no. refers to the hydrochloride. Prodrug of levodopa.

Et ester: ***Etilevodopa, USAN***
[37178-37-3]
$C_{11}H_{15}NO_4$ 225.244
Sol. prodrug of levodopa.

Et ester, hydrochloride: [39740-30-2]
Cryst. (Et_2O/EtOH). Mp 126-129°. $[\alpha]_D^{22}$ -8.95 (c, 1.05 in H_2O).

N-*Ac:* N-*Acetyl-3,4-dihydroxyphenylalanine*
[19641-90-8]
$C_{11}H_{13}NO_5$ 239.227
Prod. by *Streptomyces akiyoshiensis* ATCC13480. Sol. H_2O, MeOH. $[\alpha]_D^{20}$ +68.2 (c, 1 in MeOH). λ_{max} 198 (ϵ 34200); 280 (ϵ 2210) (H_2O) (Berdy).

O,O,N-*Tribenzoyl:* [97857-68-6]
$C_{30}H_{23}NO_7$ 509.514
Needles (AcOH). Mp 170°.

N-*(4-Hydroxy-*E*-cinnamoyl):* **N-trans-p-*Coumaroyl-DOPA***
[77201-64-0]
$C_{18}H_{17}NO_6$ 343.335
Constit. of the bark of *Dalbergia melanoxylon* and of roasted cocoa powder.

N-*(4-Hydroxy-*Z*-cinnamoyl):* **N-cis-p-*Coumaroyl-DOPA***
[77201-63-9]
$C_{18}H_{17}NO_6$ 343.335
Constit. of the bark of *Dalbergia melanoxylon.*

N-*(4-Methylbenzenesulfonyl):* [37169-34-9]
$C_{16}H_{17}NO_6S$ 351.379
Cryst. (EtOAc/petrol). Mp 188°. $[\alpha]_D^{25}$ -5.4 (c, 1 in MeOH).

N-tert-*Butyloxycarbonyl:* [30033-24-0]
$C_{14}H_{19}NO_6$ 297.307
Solid (EtOAc/cyclohexane). Mp 148° (142-144°). $[\alpha]_D^{25}$ +16.4 (c, 1 in MeOH).

N-tert-*Butyloxycarbonyl, Me ester:*
[37169-36-1]
$C_{15}H_{21}NO_6$ 311.334
Solid (MeOH aq.). Mp 140-141° (133-135°). $[\alpha]_D^{25}$ +12.3 (c, 1 in MeOH) (+7.6).

N-tert-*Butyloxycarbonyl, benzyl ester:*
[37169-37-2]
$C_{21}H_{25}NO_6$ 387.432
Brown glass. $[\alpha]_D^{25}$ -4.2 (c, 1 in MeOH).

N-*(9-Fluorenylmethyloxycarbonyl): Fmoc-L-DOPA*
[137018-93-0]
$C_{24}H_{21}NO_6$ 419.433
Solid.

N,N,N-*Tri-Me, betaine: α-Carboxy-3,4-dihydroxy-*N,N,N-*trimethylbenzeneethanaminium(1+). DOPA betaine*
[81130-72-5]
$C_{12}H_{18}NO_4^{\oplus}$ 240.279
Constit. of *Lobaria laetevirens.*

N,N,N-*Tri-Me, Me ester: 3,4-Dihydroxy-α-(methoxycarbonyl)-*N,N,N-*trimethylbenzeneethanaminium(1+), 9CI.* ***Sticticin***
[77035-53-1]
$C_{13}H_{20}NO_4^{\oplus}$ 254.305
Isol. from the thallus of *Lobaria laetevirens* and present in other lichens of the Stictaceae. V. hygroscopic solid (as chloride).

3′-Me ether: 4-Hydroxy-3-methoxyphenylalanine. 3-Methoxytyrosine
[300-48-1]
$C_{10}H_{13}NO_4$ 211.217
Isol. from *Cortinarius brunneus, Pachymatisma johnstoni* and the blood of Parkinsonian patients. Cryst. (H_2O). $[\alpha]_D$ -34 (c, 0.39 in H_2O). $[\alpha]_D$ -15.4 (c, 0.36 in 0.1*M* HCl).

5,5′-Dimer: α,α′-Diamino-5,5′,6,6′-tetrahydroxy-3,3′-biphenyldipropanoic acid, 8CI
[17785-52-3]
$C_{18}H_{20}N_2O_8$ 392.365
Powder (H_2O containing SO_2). Mp 300°.

N-*Jasmonoyl:* **N-*Jasmonoyl DOPA***
[866421-54-7]
$C_{21}H_{27}NO_6$ 389.447
Constit. of the flowers of *Vicia faba* (broad bean).

(±)*-form* [63-84-3]
Cryst. (H_2O or $NaHSO_3$ aq.). Mp 271-272° dec.

▶ AY5250000

Hydrochloride: [63302-79-4]
Plates (MeOH). Mp 246° dec.

Hydrobromide:
Plates (MeOH). Mp 212° dec.

Me ester: [41439-83-2]
Mp 126°.

Me ester, hydrochloride: [40611-00-5]
Mp 180-181°.

Et ester: [23234-42-6]
Cryst. (EtOH aq.). Mp 129°.

O,O,N-*Tri-Ac:* [47302-76-1]
$C_{15}H_{17}NO_7$ 323.302
Prisms (H_2O). Mp 171-172°.

N-*Benzoyl:* [38250-04-3]
$C_{16}H_{15}NO_5$ 301.298
Cryst. Mp 190-195° (anhyd.).

N-tert-*Butyloxycarbonyl:* [59686-55-4]
Solid (EtOAc/C_6H_6). Mp 140-142°.

N-tert-*Butyloxycarbonyl, Me ester:*
[59686-54-3]
Solid (MeOH aq.). Mp 186-188°.

N-tert-*Butyloxycarbonyl, di-Ac:* [59686-56-5]
$C_{18}H_{23}NO_8$ 381.382
Solid. Mp 132-134°.

3′-Me ether: [4214-13-5]
Prisms + $2H_2O$ (H_2O). Mp 255-256° dec.

3′-Me ether, N-*benzoyl:* [2901-78-2]
$C_{17}H_{17}NO_5$ 315.325
Plates (H_2O or EtOH). Mp 164°.

3′,4′-Di-Me ether: [33522-62-2]
$C_{11}H_{15}NO_4$ 225.244
Needles (EtOH aq.). Mp 252-255°.

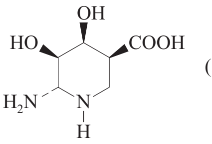
3′,4′-Di-Me ether, N-*benzoyl:* [34996-90-2]
$C_{18}H_{19}NO_5$ 329.352

Mp 173-174°.

[57308-51-7 , 127441-81-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 257A; 257B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1190A; 1190B (*nmr*)
O'Neill, J.J. *et al., J.O.C.*, 1956, **21**, 363-364 (*Me ester*)
Losse, G. *et al., Chem. Ber.*, 1961, **94**, 2271-2277 (*Et ester, synth*)
Andrews, R.S. *et al., Nature (London)*, 1965, **205**, 1213 (*glucoside*)
Kaiser, A. *et al., Helv. Chim. Acta*, 1970, **53**, 1708-1712 (*N-Ac, Boc-L-DOPA, synth, pmr*)
Chapman, R.F. *et al., J.C.S.(C)*, 1970, 865 (*dimer*)
Vorbruggen, H. *et al., Chem. Ber.*, 1972, **105**, 1168 (*synth*)
Ger. Pat., 1972, 2 153 811; *CA*, **77**, 62311a (*Boc derivs*)
Griffith, T. *et al., Phytochemistry*, 1973, **12**, 1651 (*biosynth*)
Mostad, A. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 1161 (*cryst struct*)
Renth, E.-O. *et al., Angew. Chem., Int. Ed.*, 1975, **14**, 361 (*synth*)
Fellman, J.H. *et al., Biochim. Biophys. Acta*, 1975, **381**, 9 (*isol, deriv*)
Bartholini, G. *et al., Pharmacol. Ther., Part B*, 1975, **1**, 407 (*rev, pharmacol*)
Gomez, R. *et al., Anal. Profiles Drug Subst.*, 1976, **5**, 189 (*rev*)
Bannerjee, S.N. *et al., J.O.C.*, 1976, **41**, 3056-3058 (*Boc derivs*)
Boder, N. *et al., J. Med. Chem.*, 1977, **20**, 1435-1445 (*S-form Me ester, synth, pmr*)
Dardenne, G. *et al., Phytochemistry*, 1977, **16**, 1822 (*deriv*)
Yamamoto, H. *et al., Polymer*, 1977, **18**, 979; 1978, **19**, 1115 (*polym*)
Fuller, W.D. *et al., Biopolymers*, 1978, **17**, 2939 (*polym*)
Rudd, E.A. *et al., J. Med. Chem.*, 1979, **22**, 233-237 (*Boc-L-DOPA Me ester*)
Bernard, T. *et al., Phytochemistry*, 1980, **19**, 1967 (*Sticticin*)
Van Heerden, F.R. *et al., Phytochemistry*, 1980, **19**, 2125 (*N-p-coumaroyl*)
Bernard, T. *et al., Phytochemistry*, 1981, **20**, 2325 (*betaine*)
Danishevsky, S. *et al., Tetrahedron*, 1981, **37**, 4081 (*synth*)
Nutt, J.G. *et al., Clin. Neuropharmacol.*, 1984, **7**, 35 (*rev, metab*)
Laycock, M.V. *et al., J. Nat. Prod.*, 1984, **47**, 1033 (*isol, sulfate*)
Lee, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 235 (*hplc, bibl, anal*)
Cooper, D.R. *et al., J. Pharm. Pharmacol.*, 1987, **39**, 627-635; 809-818 (*Et ester*)
Behrman, E.J. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 351 (*synth, sulfate*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag*, 1994, 1471 (*synonyms*)
Smith, K.C. *et al., J. Nat. Prod.*, 1995, **58**, 1274 (*isol, N-Ac*)
Brunner-Guenat, M. *et al., J. Pharm. Pharmacol.*, 1995, **47**, 861 (*Me ester*)
Djaldetti, R. *et al., Ann. Neurol.*, 1996, **39**, 400-404 (*Et ester*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1137
Chen, F.-Y. *et al., J.O.C.*, 2001, **66**, 3650-3652 (*R-form, ir, pmr, cmr*)
Sever, M.J. *et al., Tetrahedron*, 2001, **57**, 6139-6146 (*Fmoc/TBDMS derivs*)
Kramell, R. *et al., J. Nat. Prod.*, 2005, **68**, 1345-1349 (*N-jasmonoyl*)
Stark, T. *et al., J. Agric. Food Chem.*, 2006, **54**, 2859-2867 (*N-4-hydroxycinnamoyl, isol*)
Aubry, S. *et al., Eur. J. Org. Chem.*, 2007, 5212-5225 (*S-form, Me ester*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DNA200

6-Amino-4,5-dihydroxy-3-piperidinecarboxylic acid A-746



(3*S*,4*S*,5*R*,6*S*)–*form*

$C_6H_{12}N_2O_4$ 176.172

(3S,4S,5R,6S)-form

N-*Ac:* ***Siastatin B***. *A 72363B. Antibiotic A 72363B*
[54795-58-3]
$C_8H_{14}N_2O_5$ 218.209
Isol. from *Streptomyces verticillus* var. *quintum* and *Streptomyces nobilis*. Potent neuraminidase inhibitor. Needles. Mp 137° dec. $[\alpha]_D^{25}$ +57.2 (c, 1 in H_2O).

▸TM6125400

(3R*,4R*,5R*,6R*)-form

N-*Ac:* ***Antibiotic A 72363A1***. *A 72363A-1*
$C_8H_{14}N_2O_5$ 218.209
Prod. by *Streptomyces nobilis*. Heparanase inhibitor. Sol. H_2O; poorly sol. Me_2CO, hexane. $[\alpha]_D^{23}$ +29 (c, 1 in H_2O).

(3R*,4S*,5R*,6R*)-form

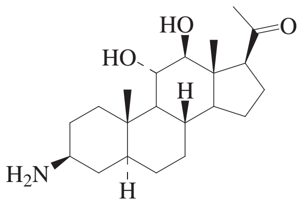
N-*Ac:* ***Antibiotic A 72363A2***. *A 72363A-2*
$C_8H_{14}N_2O_5$ 218.209
Prod. by *Streptomyces nobilis*. Heparanase inhibitor. Sol. H_2O; poorly sol. Me_2CO, hexane. $[\alpha]_D^{23}$ -31 (c, 1 in H_2O).

(3R*,4R*,5S*,6S*)-form

N-*Ac:* ***Antibiotic A 72363C***. *A 72363C*
$C_8H_{14}N_2O_5$ 218.209
Prod. by *Streptomyces nobilis*. Heparanase inhibitor. Sol. H_2O; poorly sol. Me_2CO, hexane. $[\alpha]_D^{27}$ -59 (c, 0.7 in H_2O).

Umezawa, H. *et al., J. Antibiot.*, 1974, **27**, 963 (*isol, ir, props*)
Aoyagi, T. *et al., Experientia*, 1975, **31**, 896 (*struct*)
Nishimura, Y. *et al., J.A.C.S.*, 1988, **110**, 7249 (*synth, abs config*)
Nishimura, Y. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 978 (*synth*)
Nishimura, Y. *et al., Stud. Nat. Prod. Chem.*, 1995, **16**, 75 (*rev, synth*)
Takatsu, T. *et al., J. Antibiot.*, 1996, **49**, 54; 61 (*A 73263, pmr, cmr, activity*)
Knapp, S. *et al., Org. Lett.*, 2000, **2**, 4037-4040 (*Siastatin B, synth*)

3-Amino-11,12-dihydroxypregnan-20-one A-747



$C_{21}H_{35}NO_3$ 349.512

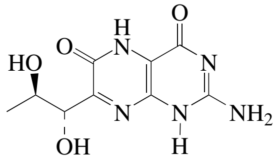
(3β,5α,11α,12β)-form

N,N-*Di-Me, 11-*O*-(3,4-dimethyl-3-pentenoyl), 12-Ac:* ***Pachysanonin***
[873799-27-0]
$C_{32}H_{51}NO_5$ 529.759
Constit. of *Pachysandra axillaris*. Cryst. (Me_2CO). Mp 153.5-154.5°.

Qiu, M.-H. *et al., Chem. Biodiversity*, 2005, **2**, 866-871 (*Pachysanonin*)

2-Amino-7-(1,2-dihydroxypropyl)-1,5-dihydro-4,6-pteridinedione, 9CI A-748

6-Oxoprimapterin. *6-Oxo-7-biopterin*
[115991-76-9]

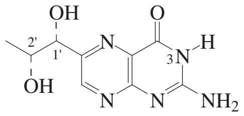


$C_9H_{11}N_5O_4$ 253.217
Occurs in the urine of humans with hyperphenylalaninemia.

Curtuis, H.C. *et al., J. Biol. Chem.*, 1990, **265**, 3923-3930 (*isol, ms, struct*)

2-Amino-6-(1,2-dihydroxypropyl)-4(1*H*)-pteridinone A-749

2-Amino-4-hydroxy-6-(1,2-dihydroxypropyl)pterin



(1′*R*,2′*R*)-*form*

$C_9H_{11}N_5O_3$ 237.218

(1′R,2′R)-form

D-threo-*form*. ***Dictyopterin***
[13019-52-8]
Isol. from *Dictyostelium discoideum*. Mp 300°. pK_{a1} 2.2; pK_{a2} 7.92.

(1′R,2′S)-form

L-erythro-*form*. ***Biopterin***. *Ranachrome 1*
[22150-76-1]
Widely distributed in microorganisms, insects, algae, amphibia and mammals. Found in urine. Growth factor. Pale yellow cryst. (AcOH aq.). Mp 250-280° dec. $[\alpha]_D^{20}$ -66 (c, 0.2 in 0.1*M* HCl). pK_{a1} 2.23; pK_{a2} 7.89.

▸UO3506000

*1′-*O*-D-Glucopyranoside: Biopterin glucose*
[32838-67-8]
$C_{15}H_{21}N_5O_8$ 399.36
Constit. of a marine plankton.

*2′-*O*-α-D-Glucopyranoside:* [235416-12-3]
$C_{15}H_{21}N_5O_8$ 399.36
Isol. from *Spirulina* (*Arthrospira*) *platensis.*

*2′-*O*-(2-Acetamido-2-deoxy-β-D-glucopyranoside):* ***Limipterin***

[164803-20-7]
$C_{17}H_{24}N_6O_8$ 440.412
Prod. by *Chlorobium limicola f. thiosulfatophilum*.

3-Me: ***2-Amino-6-(1,2-dihydroxypropyl)-3-methylpterin-4-one***
[111317-37-4]
$C_{10}H_{13}N_5O_3$ 251.244
Isol. from the marine anthozoan *Astroides calycularis*. Pale yellow cryst. powder (MeOH). Sol. MeOH, H_2O. Mp 229-231°. $[\alpha]_D$ -60 (c, 0.3 in 0.1*M* HCl). λ_{max} 230 (ϵ 28200); 319 (ϵ 11700) (pH 1 H_2O) (Derep). λ_{max} 242 (ϵ 28200); 276 (ϵ 24000); 356 (ϵ 9550) (H_2O pH 7) (Derep).

7,8-Dihydro: 7,8-Dihydrobiopterin
[6779-87-9]
[7644-44-2]
$C_9H_{13}N_5O_3$ 239.233
Hygroscopic needles (H_2O or MeOH aq.). $[\alpha]_D^{22}$ +35 (c, 0.4 in 0.1*M* NaOH).

5,6,7,8-Tetrahydro: see 5,6,7,8-Tetrahydrobiopterin, T-142

(1′*S*,2′*R*)-*form*
D-erythro-*form*
[13039-62-8]
Mp 300°. pK_{a1} 2.23; pK_{a2} 7.9.

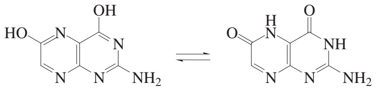
(1′*S*,2′*S*)-*form*
L-threo-*form*. ***Orinapterin***. *Ciliapterin*
[13039-82-2]
Isol. from human urine. Prod. by *Aphanizomenon flos-aquae*. Pale yellow cryst. (AcOH aq.). Mp 300°. $[\alpha]_D$ +72 (0.1*M* HCl). pK_{a1} 2.24; pK_{a2} 7.87.

2′-O-(2-Acetamido-2-deoxy-β-D-glucopyranoside): ***Tepidopterin***
[188778-28-1]
$C_{17}H_{24}N_6O_8$ 440.412
Prod. by *Chlorobium tepidum*.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 480B (*nmr*)
Patterson, E.L. *et al., J.A.C.S.*, 1955, **77**, 3167
Kidder, G.W. *et al., J. Biol. Chem.*, 1968, **243**, 826 (*Ciliapterin*)
Kidder, G.W. *et al., Methods Enzymol.*, 1971, **18B**, 739 (*Ciliapterin*)
Rembold, H. *et al., Angew. Chem., Int. Ed.*, 1972, **11**, 1061 (*biochem*)
Blair, J.A. *et al., Tet. Lett.*, 1973, 203-204 (*synth, uv, dihydro*)
Sugimoto, T. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 3767 (*synth*)
Taylor, E.C. *et al., J.A.C.S.*, 1976, **98**, 2301 (*synth*)
Schircks, B. *et al., Helv. Chim. Acta*, 1977, **60**, 211; 1978, **61**, 2731-2738; 1985, **68**, 1639 (*synth, pmr, cmr, derivs*)
Fukushima, T. *et al., Methods Enzymol.*, 1980, **66**, 508-511 (*synth, uv, dihydro*)
Armarego, W.L.F. *et al., Aust. J. Chem.*, 1982, **35**, 785 (*synth*)
Kappel, M. *et al., Annalen*, 1984, 1815 (*synth*)
Aiello, A. *et al., Experientia*, 1987, **43**, 950 (*deriv*)
Mori, K. *et al., Annalen*, 1989, 958; 1212 (*synth, bibl*)
Klein, R. *et al., Eur. J. Biochem.*, 1990, **187**, 665 (*Dictyopterin*)
Ogiwara, S. *et al., Biol. Chem. Hoppe-Seyler*, 1992, **373**, 1061 (*Orinapterin*)
Cha, K.W. *et al., Helv. Chim. Acta*, 1995, **78**, 600-614 (*Limipterin*)
Ikawa, M. *et al., Phytochemistry*, 1995, **38**, 1229 (*isol, pmr, ms*)
Fernandez, A.M. *et al., J.O.C.*, 1996, **61**, 8698 (*synth*)
Cho, S.-H. *et al., Biochim. Biophys. Acta*, 1998, **1379**, 53-60 (*Tepidopterin*)
Noguchi, Y. *et al., Mar. Biotechnol.*, 1999, **1**, 207-210 (*2′-glucoside*)
Hanaya, T. *et al., Tetrahedron*, 2008, **64**, 2090-2100 (*Limipterin, Tepidopterin, synth*)

2-Amino-4,6-dihydroxypteridine A-750

2-Amino-1,5-dihydro-4,6-pteridinedione, 9CI. ***Xanthopterin***. *Uropterin*
[119-44-8]
[5979-01-1]



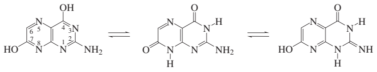
$C_6H_5N_5O_2$ 179.138
Important naturally occurring pteridine. Normal constit. of human urine. Yellow wing pigment of butterflies e.g. *Gonepteryx rhamni*, *Appias nero*, *Colias edusa*. Inhibits cell proliferation. Sol. acids, alkalis. Mp 410° (carbonises above 360°). pK_{a1} 6.25; pK_{a2} 9.23 (20°).

6-O-Sulfate: ***Xanthopterinsulfonic acid***
$C_6H_5N_5O_5S$ 259.202
Prod. by *Azotomonas insolita* and *Escherichia coli*. Needles (H_2O) (as Na salt). Mp 300° (Na salt).

Schöpf, C. *et al., Annalen*, 1933, **507**, 266
Goto, M. *et al., Arch. Biochem. Biophys.*, 1965, **111**, 8 (*Xanthopterinsulfonic acid*)
Taylor, E.C. *et al., J.A.C.S.*, 1973, **95**, 4455 (*synth*)
Bieri, J.H. *et al., Helv. Chim. Acta*, 1976, **59**, 2374 (*cryst struct*)
Pfleiderer, W. *et al., J. Het. Chem.*, 1992, **29**, 583 (*rev*)
Rubenstein, M. *et al., Int. J. Biochem.*, 1993, **25**, 1873

2-Amino-4,7-dihydroxypteridine A-751

*2-Amino-4,7(1*H*,8*H*)-pteridinedione, 9CI.* ***Isoxanthopterin***. *Ranachrome 4*
[529-69-1]



$C_6H_5N_5O_2$ 179.138
Widespread insect pigment found in amphibian and fish skin; normal constit. of urine. Mp 300°. pK_{a1} 7.34; pK_{a2} 10.06 (20°,H_2O).

▶ UO3425000

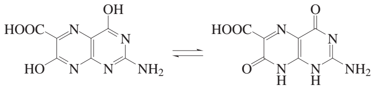
1*H*,3*H*-*form*

Me ether, 1,3-di-Me: **N^1,N^3,O^7-*Trimethylisoxanthopterin***
$C_9H_{11}N_5O_2$ 221.218
Isol. from a *Eudistoma* sp. Solid. λ_{max} 208 (sh) (log ϵ 4); 236 (sh) (log ϵ 3.7); 268 (log ϵ 3.4); 316 (log ϵ 3.6); 328 (sh) (log ϵ 3.6); 350 (sh) (log ϵ 3) (MeOH).

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 769A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 895D (*ir*)
Pfleiderer, W. *et al., Chem. Ber.*, 1961, **94**, 1 (*struct, bibl, uv*)
Konrad, G. *et al., Chem. Ber.*, 1970, **103**, 735 (*uv, props*)
Taylor, E.C. *et al., J.O.C.*, 1975, **40**, 2341 (*synth, bibl*)
Pfleiderer, W. *et al., J. Het. Chem.*, 1992, **29**, 583 (*rev*)
Van Wagoner, R.M. *et al., J. Nat. Prod.*, 2001, **64**, 1100-1101 (*N,N,O-trimethyl*)

2-Amino-4,7-dihydroxy-6-pteridinecarboxylic acid A-752

2-Amino-1,4,7,8-tetrahydro-4,7-dioxo-6-pteridinecarboxylic acid, 9CI. ***Isoxanthopterincarboxylic acid, 8CI***. *Cyprino-Pourpre B*
[3254-85-1]

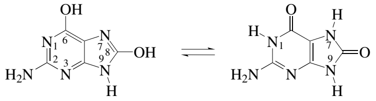


$C_7H_5N_5O_4$ 223.148
Isol. from the scales and skin of various fish. Cryst. Mp > 360°. λ_{max} 224 (log ϵ 4.57); 259 (log ϵ 4); 282 (sh) (log ϵ 3.53); 347 (log ϵ 4.17) (0.1*M* NaOH).

Purrmann, R *et al., Annalen*, 1941, **548**, 284-292 (*synth*)
Matsuura, S *et al., J. Biochem. (Tokyo)*, 1955, **42**, 419-422 (*isol*)
Taylor, E.C. *et al., J.A.C.S.*, 1959, **81**, 2474-2479 (*synth*)
Taylor, E.C *et al., Tet. Lett.*, 1973, 2093-2095 (*synth*)

2-Amino-6,8-dihydroxypurine A-753

*2-Amino-7,9-dihydro-1*H*-purine-6,8-dione, 9CI. 8-Oxoguanine. 7,8-Dihydro-8-oxoguanine. 2-Aminopurine-6,8-diol. 8-Hydroxyguanine*
[5614-64-2]



$C_5H_5N_5O_2$ 167.127
Other tautomers possible. 8-Oxo form predominates. Prod. *in vivo* by free radical hydroxylations of guanine radicals in DNA. Involved in base pair mismatches in mutagenesis. Crystalline powder. Mp 300°.

▶ Potent mutagen.

7-Me: 2-Amino-6,8-dihydroxy-7-methylpurine. 2-Amino-7-methyl-6,8-purinediol. 8-Hydroxy-7-methylguanine
[1688-85-3]
$C_6H_7N_5O_2$ 181.154
Platelets.

*9-Me: 2-Amino-6,8-dihydroxy-9-methylpurine. 2-Amino-9-methyl-6,8-purinediol. 8-Hydroxy-9-methylguanine. 9-Methylguanin-8(7*H*)-one*
[21823-84-7]
$C_6H_7N_5O_2$ 181.154
Cryst. + H_2O. Mp 400°.

*1,7-Di-Me: 1,7-Dimethyl-8-oxo-9*H*-guanine*
[65879-11-0]
$C_7H_9N_5O_2$ 195.18
Cryst. (H_2O). Gradual dec. >240°.

7,O^6-Di-Me: ***2-Amino-8-hydroxy-6-methoxy-7-methylpurine****. 2-Amino-7,9-dihydro-6-methoxy-7-methyl-8*H*-purin-8-one. 6-Methoxy-7-methyl-8-oxoguanine*
[247165-80-6]
$C_7H_9N_5O_2$ 195.18
Isol. from the ascidian *Symplegma rubra*. Solid. λ_{max} 210 (log ϵ 4.2); 246 (log ϵ 3.6); 284 (log ϵ 3.9) (MeOH).

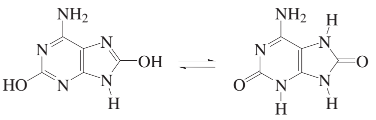
*9-Et: 2-Amino-9-ethyl-6,8-dihydroxypurine. 2-Amino-9-ethyl-6,8(1*H*,9*H*)-purinedione*
[21823-85-8]
$C_7H_9N_5O_2$ 195.18
Cryst. (KOH aq./AcOH). Mp 359-360°.

[112009-08-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 716D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 217C (*nmr*)
Fischer, E. *et al., Ber.*, 1897, **30**, 570 (*synth*)
Karrer, P. *et al., Helv. Chim. Acta*, 1948, **31**, 1214 (*isol*)
Cavalieri, L.F. *et al., J.A.C.S.*, 1950, **72**, 2587 (*synth, uv*)
Borowitz, I.J. *et al., Biochemistry*, 1965, **4**, 650 (*7-Me*)
Perini, F. *et al., J.O.C.*, 1970, **35**, 812 (*synth, uv, derivs*)
Brown, R. *et al., J.C.S. Perkin 1*, 1977, 1003 (*9-Me*)
Parham, J.C. *et al., J.O.C.*, 1978, **43**, 2325 (*di-Me*)
Dizdaroglu, M. *et al., Biochemistry*, 1985, **24**, 4476 (*formn*)
Kohda, K. *et al., Biochem. Biophys. Res. Commun.*, 1987, **149**, 1141 (*formn*)
Kasai, H. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 3799 (*cryst struct, 9-Et*)
Floyd, R.A. *et al., Carcinogenesis (London)*, 1990, **11**, 1447 (*rev*)
Doi, M. *et al., J.C.S. Perkin 1*, 1991, 55 (*cryst struct, 9-Et*)
Brown, T. *et al., Chem. Ber.*, 1993, 484 (*rev*)
Linday, B.S. *et al., J. Nat. Prod.*, 1999, **62**, 1573-1575 (*2-Amino-8-hydroxy-6-methoxy-7-methylpurine*)

6-Amino-2,8-dihydroxypurine A-754

*6-Amino-1*H*-purine-2,8(3*H*,7*H*)-dione, 9CI. 6-Aminopurine-2,8-diol. 2,8-Dihydroxyadenine*
[30377-37-8]



$C_5H_5N_5O_2$ 167.127
Other tautomers possible. Prod. by *Alcaligenes aquamarinus*. Found in urine of humans with 2,8-dihydroxyadenine urolithiasis associated with adenine phosphoribosyltransferase deficiency. Xanthine oxidase inhibitor. Sol. bases; fairly sol. H_2O; poorly sol. MeOH, DMSO, hexane. Mp 335-340° dec. λ_{max} 305 (ϵ 19950) (HCl) (Berdy). λ_{max} 300 (ϵ 14800) (NaOH) (Berdy).

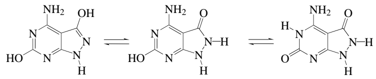
(1*H*,3*H*)-form

*1,3-Di-Me: 6-Amino-1,3-dimethyl-1*H*-purine-2,8(3*H*,8*H*)-dione. 1,3-Dimethyl-8-oxoisoguanine*
[683228-71-9]
$C_7H_9N_5O_2$ 195.18
Isol. from the ascidian *Pseudodistoma cereum* and from *Phestilla melanobtanchia* and a *Tubastrea* sp. Amorph. solid. λ_{max} 203 (log ϵ 3.89); 308 (log ϵ 3.57) (MeOH).

Bendich, A. *et al., J. Biol. Chem.*, 1950, **183**, 267-277 (*isol*)
Cavalieri, L.F. *et al., J.A.C.S.*, 1950, **72**, 2587-2594 (*synth*)
Klenow, H. *et al., Biochem. J.*, 1952, **50**, 404-407 (*isol*)
Stevens, M.A. *et al., J.A.C.S.*, 1960, **82**, 1148-1152 (*synth*)
Simmonds, H.A. *et al., Biochem. J.*, 1976, **157**, 485-487 (*isol*)
Sunahara, N. *et al., Agric. Biol. Chem.*, 1977, **41**, 1103-1109 (*isol*)
Simmonds, H.A. *et al., Clin. Chim. Acta*, 1986, **160**, 103-108 (*biochem, rev*)
Kamatani, N. *et al., Pharma Med.*, 1988, **6**, 39-42 (*rev*)
Kojima, T. *et al., Biomed. Chromatogr.*, 1991, **5**, 57-61 (*hplc*)
Simmonds, H.A. *et al., Lancet*, 1992, **ii**, 1295-1296 (*biochem*)
Sumi, S. *et al., J. Chromatogr., B*, 1995, **672**, 233-239 (*hplc*)
Sevcik, J. *et al., Clin. Chim. Acta*, 1996, **245**, 85-92 (*occur*)
Engle, S.J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1996, **93**, 5307-5312 (*biochem*)
Appleton, D.R. *et al., Nat. Prod. Res.*, 2004, **18**, 39-42 (*1,3-di-Me*)

4-Amino-3,6-dihydroxy-1*H*-pyrazolo[3,4-*d*]pyrimidine A-755

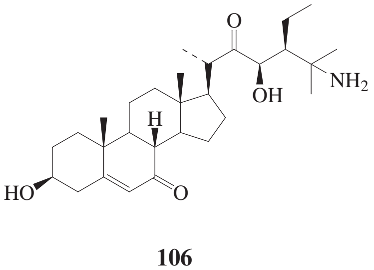
*4-Amino-1*H*-pyrazolo[3,4-*d*]pyrimidine-3,6(2*H*,5*H*)-dione, 9CI.* ***Hydroxyakalone***
[182056-35-5]



$C_5H_5N_5O_2$ 167.127
Prod. by the marine *Agrobacterium aurantiacum*. Xanthine oxidase inhibitor. Shows antigout activity. Powder. Sol. bases, DMSO; poorly sol. MeOH, hexane, $CHCl_3$. λ_{max} 298 (H_2O). λ_{max} 298 (pH12 buffer) (Berdy).

Izumida, H. *et al., J. Antibiot.*, 1997, **50**, 916-918 (*isol, pmr, cmr*)

25-Amino-3,23-dihydroxystigmast-5-ene-7,22-dione A-756



$C_{29}H_{47}NO_4$ 473.695

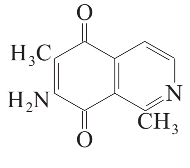
(3β,23*R*,24*S*)-form

N-Me, 3-O-β-D-glucopyranoside: ***Triumfettoside A***
[551929-44-3]
$C_{36}H_{59}NO_9$ 649.863
Alkaloid from the aerial parts of *Triumfetta flavescens*. Amorph. powder. Mp > 300°.

Ahmed, B. *et al., Pharmazie*, 2002, **57**, 709-713 (*isol, pmr, cmr, ms*)

7-Amino-1,6-dimethyl-5,8-isoquinolinedione, 9CI A-757

Cribrostatin 1
[144279-35-6]



$C_{11}H_{10}N_2O_2$ 202.212
Alkaloid from the blue marine sponge *Cribrochalina* sp. Exhibits cytotoxicity against the P388 lymphocytic leukaemia cell line. Red-orange cryst. (CH_2Cl_2/MeOH). Mp 220-235° dec. λ_{max} 207 (ϵ 8730); 232 (ϵ 4700); 256 (ϵ 4170); 272 (ϵ 4160); 304 (ϵ 537) (MeOH) (Berdy).

Pettit, G.R. *et al., Can. J. Chem.*, 1992, **70**, 1170 (*isol, uv, ir, pmr, cmr, cryst struct*)

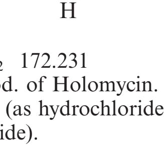
2-Amino-14,16-dimethyl-3-octadecanol A-758

Paecilaminol*. Antibiotic FKI 0550. FKI 0550*
$H_3CCH_2CH(CH_3)CH_2CH(CH_3)(CH_2)_{10}CH(OH)CH(NH_2)CH_3$
$C_{20}H_{43}NO$ 313.566
Prod. by *Fusarium avenaceum* and *Paecilomyces* sp. FKI-0550. NADH-fumarate reductase inhibitor. Cytotoxic. Mycotoxin. Pale yellow oil. $[\alpha]^{25}_{D}$ +26.7 (c, 0.24 in MeOH). λ_{max} 203 (ϵ 8250); 220 (sh) (ϵ 4400); 246 (ϵ 2040); 265 (sh) (ϵ 1570) (MeOH).

Uhlig, S. *et al., Toxicon*, 2005, **46**, 513-522 (*isol, pmr, cmr, ms*)
Ui, H. *et al., J. Antibiot.*, 2006, **59**, 591-596 (*isol, pmr, cmr, activity*)

6-Amino-1,2-dithiolo[4,3-*b*]pyrrol-5(4*H*)-one, 9CI A-759

Holothin
[488-03-9]



$C_5H_4N_2OS_2$ 172.231
Hydrol. prod. of Holomycin. Greenish-black cryst. (as hydrochloride). Mp 300° (hydrochloride).

▶AB7450000

N^6-Ac: ***Holomycin****. N-Demethylthiolutin.*

Antibiotic MM 21801. MM 21801
[488-04-0]
$C_7H_6N_2O_2S_2$ 214.269
Prod. by *Streptomyces* sp. P6621 and *Streptomyces clavuligerus*. Shows antibiotic props. Orange-yellow flakes (MeOH/EtOAc). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 268-270° dec. λ_{max} 246 (ε 6460); 302 (ε 3090); 388 (ε 11200) (MeOH or EtOH) (Derep). λ_{max} 246 (ε 4665); 301 (ε 2354); 388 (ε 7918) (MeOH) (Berdy). λ_{max} 245 (ε 6310); 302 (ε 3310); 390 (ε 11750) (EtOH) (Berdy).

▶ AB7450000

N^6*-Propanoyl:* ***N-Propionylholothin***. *N-(4,5-Dihydro-5-oxo-1,2-dithiolo[4,3-*b*]-pyrrol-6-yl)propanamide, 9CI*
[4708-23-0]
$C_8H_8N_2O_2S_2$ 228.295
Isol. from *Streptomyces* P6621. Orange-yellow prisms. Sol. MeOH. Mp 255-264° dec. λ_{max} 246 (ε 6460); 302 (ε 3090); 388 (ε 11200) (MeOH or EtOH) (Derep). λ_{max} 246 (ε 7800); 302 (ε 4250); 388 (ε 14400) (MeOH) (Berdy).

N^6*-Hexanoyl:* ***Xenorhabdin 1***. *N-(4,5-Dihydro-5-oxo-1,2-dithiolo[4,3-*b*]pyrrol-6-yl)hexanamide, 9CI*
[92680-94-9]
$C_{11}H_{14}N_2O_2S_2$ 270.376
Prod. by *Xenorhabdus* spp. Possesses antimicrobial and insecticidal props. Sol. MeOH, EtOAc, DMSO; fairly sol. hexane; poorly sol. H_2O. Mp 192-193°. Related to Thiolutin and Aureothricin. λ_{max} 243 (sh) (ε 6000); 300 (ε 3100); 387 (ε 11000) (MeOH) (Derep). λ_{max} 250 ; 310 ; 390 (MeOH) (Berdy).

N^6*-Octanoyl:* ***Xenorhabdin 3***
[92680-91-6]
$C_{13}H_{18}N_2O_2S_2$ 298.429
Prod. by *Xenorhabdus* spp. Possesses antimicrobial and insecticidal props. Sol. MeOH, DMSO, EtOAc; fairly sol. hexane; poorly sol. H_2O. Mp 360°. λ_{max} 243 (sh) (ε 6000); 300 (ε 3100); 387 (ε 11000) (MeOH) (Derep). λ_{max} 250 ; 310 ; 390 (MeOH) (Berdy). λ_{max} 300 ; 387 (MeOH) (Berdy).

N^6*-Tetradecanoyl: N-Tetradecanoylholothin*
$C_{19}H_{30}N_2O_2S_2$ 382.59
Prod. by a marine-derived *Alteromonas* sp.

N^6*-(5-Methylhexanoyl):* ***Xenorhabdin 2***
[92680-90-5]
$C_{12}H_{16}N_2O_2S_2$ 284.403
Prod. by *Xenorhabdus* spp. Possesses antimicrobial and insecticidal props. Sol. MeOH, EtOAc, DMSO; fairly sol. hexane; poorly sol. H_2O. Mp 210-213°. λ_{max} 243 (sh) (ε 6000); 300 (ε 3100); 387 (ε 11000) (MeOH) (Derep). λ_{max} 244 ; 300 ; 387 (MeOH) (Berdy).

*4-Me: 6-Amino-4-methyl-1,2-dithiolo[4,3-*b*]pyrrol-5(4*H*)-one.* ***Pyrrothine***
[642-77-3]
$C_6H_6N_2OS_2$ 186.258
Isol. from a *Streptomyces* sp. Active against gram-positive and -negative bacteria. Amorph. yellow solid. Mp 191-194° dec.

4-Me; hydrochloride:
Yellow prisms + $1H_2O$. Sinters at *ca.* 200°.

4-Me, N^6*-Ac:* ***Thiolutin***. *N-Acetylpyrrothine. Farcinicine*†. *Acetopyrrothine*
[87-11-6]
$C_8H_8N_2O_2S_2$ 228.295
Prod. by *Streptomyces albus*, *Streptomyces pimprina*, *Streptomyces thioluteus*, other *Streptomyces* spp. and *Saccharothrix* sp. SA 233. Antibiotic which inhibits microbiological growth in beer. Phytotoxic in high concentrations. Shows platelet aggregation props. Brilliant yellow needles (1-butanol). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, C_6H_6, Et_2O, hexane. Mp 273-276° dec. $Bp_{0.1}$ 200° subl. λ_{max} 248 (ε 6300); 311 (ε 5700); 388 (ε 10800) (MeOH) (Derep). λ_{max} 250 (ε 6030); 311 (ε 5600); 388 (ε 10960) (MeOH) (Berdy).

▶ LD_{50} (mus, scu) 25 mg/kg. JP1355000

4-Me, N^6*-propanoyl:* ***Aureothricin***. *Propionylpyrrothine. Farcinicin*†
[574-95-8]
$C_9H_{10}N_2O_2S_2$ 242.322
Isol. from *Streptomyces celluloflavus* 39a, *Streptomyces cyanoflavus*, *Streptomyces kasugaensis* and *Streptomyces farcinicus*. Antibiotic and antifungal agent. Platelet aggregation inhibitor. Golden-yellow cryst. (EtOAc). Sol. MeOH, $CHCl_3$; fairly sol. C_6H_6; poorly sol. Et_2O, H_2O, hexane. Mp 260-270° dec. λ_{max} 246 (ε 6500); 313 (ε 4000); 390 (ε 11100) (EtOH) (Berdy).

▶ LD_{50} (mus, scu) 10 mg/kg.

4-Me, N^6*-butanoyl: N-(4,5-Dihydro-4-methyl-5-oxo-1,2-dithiolo[4,3-*b*]pyrrol-6-yl)butanamide.* ***N-Butanoylpyrrothine***. *Antibiotic* PSC_2. PSC_2
[112843-01-3]
$C_{10}H_{12}N_2O_2S_2$ 256.349
Prod. by *Xenorhabdus bovienii* A2 and *Saccharothrix* sp. SA 233. Yellow powder. λ_{max} 308 (log ε 3.7); 389 (log ε 3.92) (MeOH).

4-Me, N^6*-(2-methylpropanoyl): N-(2-Methylpropanoyl)pyrrothine.* ***Isobutyropyrrothine***†. *N-Isobutyrylpyrrothine. Antibiotic* PSC_1. PSC_1
[39859-18-2]
$C_{10}H_{12}N_2O_2S_2$ 256.349
Prod. by *Streptomyces pimprina* and *Saccharothrix* sp. SA 233. Shows platelet aggregation props. Orange-red plates (C_6H_6). Sol. $CHCl_3$, EtOAc, Me_2CO; fairly sol. C_6H_6; poorly sol. H_2O, hexane. Mp 228-229°. λ_{max} 245 ; 290 ; 310 ; 388 (MeOH) (Berdy). λ_{max} 246 (ε 5400); 302 (ε 3000); 386 (ε 11000) (MeOH) (Derep).

4-Me, N^6*-hexanoyl:* ***Xenorhabdin 4***. *N-Pentanoylpyrrothine*
[92680-92-7]
$C_{12}H_{16}N_2O_2S_2$ 284.403
From *Xenorhabdus* spp. Possesses antimicrobial and insecticidal props. Sol. MeOH, DMSO, EtOAc; fairly sol. hexane; poorly sol. H_2O. Mp 165°. λ_{max} 246 (sh) (ε 6300); 308 (ε 5700); 388 (ε 11000) (MeOH) (Derep). λ_{max} 245 ; 310 (ε 1000); 312 ; 390 (ε 10000) (MeOH) (Berdy).

4-Me, N^6*-(3-methylbutanoyl): N-(4,5-Dihydro-4-methyl-5-oxo-1,2-dithiolo[4,3-*b*]pyrrol-6-yl)-3-methylbutanamide.* ***N-(3-Methylbutanoyl)pyrrothine***
[167559-98-0]
$C_{11}H_{14}N_2O_2S_2$ 270.376
Isol. from *Xenorhabdus bovienii* A2. Solid.

4-Me, N^6*-(5-methylhexanoyl): N-(5-Methylhexanoyl)pyrrothine.* ***Xenorhabdin 5***
[92680-93-8]
$C_{13}H_{18}N_2O_2S_2$ 298.429
From *Xenorhabdus* spp. Possesses antimicrobial and insecticidal props. Sol. MeOH, EtOAc, DMSO; fairly sol. hexane; poorly sol. H_2O. λ_{max} 246 (sh) (ε 6300); 308 (ε 5700); 388 (ε 11000) (MeOH) (Derep). λ_{max} 246 ; 250 ; 308 ; 310 (ε 1000); 388 ; 390 (ε 10000) (MeOH) (Berdy).

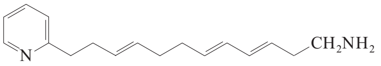
4-Me, N^6*-(3-methyl-2-butenoyl):* ***N-Senecioylpyrrothine***. *PSA. Antibiotic PSA*
$C_{11}H_{12}N_2O_2S_2$ 268.36
Prod. by *Saccharothrix* sp. SA 233. Yellow-orange powder. λ_{max} 302 (log ε 3.87); 402 (log ε 3.97) (MeOH).

4-Me, N^6*-tigloyl:* ***N-Tigloylpyrrothine***. *PSB. Antibiotic PSB*
$C_{11}H_{12}N_2O_2S_2$ 268.36
Prod. by *Saccharothrix* sp. SA 233. Yellow-orange powder. λ_{max} 302 (log ε 3.85); 402 (log ε 3.96) (MeOH).

Celmer, W.D. *et al.*, *J.A.C.S.*, 1952, **74**, 6304; 1955, **77**, 2861 (*Pyrrothine, Aureothricin, Thiolutin, isol, ir, uv, struct*)
Ettlinger, L. *et al.*, *Helv. Chim. Acta*, 1959, **42**, 563 (*isol*)
Bhate, D.S. *et al.*, *Experientia*, 1960, **16**, 504-505 (*Isobutyropyrrothine*)
Schmidt, U. *et al.*, *Chem. Ber.*, 1964, **97**, 1511 (*synth, uv, ir*)
Büchi, G. *et al.*, *J.A.C.S.*, 1964, **86**, 5654 (*synth*)
Yamagishi, S. *et al.*, *Yakugaku Zasshi*, 1971, **91**, 351 (*Aureothicin, isol, struct, ir, pmr, ms*)
Hagio, K. *et al.*, *Bull. Chem. Soc. Jpn.*, 1974, **47**, 1484 (*Holothin, Thiolutin, Aureothricin, synth, ir, uv, pmr*)
Okamura, K. *et al.*, *J. Antibiot.*, 1977, **30**, 334-336 (*isol, ir, ms*)
Ellis, J.E. *et al.*, *J.O.C.*, 1977, **42**, 2891-2893 (*synth, ir, uv, ms, nmr*)
Kenig, M. *et al.*, *J. Antibiot.*, 1979, **32**, 549-554 (*MM 21801*)
Ninomiya, Y.T. *et al.*, *Chem. Pharm. Bull.*, 1980, **28**, 3157-3162 (*Pyrrothine, Thiolutin, props, ms*)
Deb, P.R. *et al.*, *Curr. Sci. (India)*, 1984, **53**, 659 (*Thiolutin, props*)
Pat. Coop. Treaty (WIPO), 1984, 01 775; *CA*, **101**, 189727 (*Xenorhabdins*)
McInerney, B.V. *et al.*, *J. Nat. Prod.*, 1991, **54**, 774 (*Xenorhabdins*)
Dell, I. *et al.*, *ACS Symp. Ser.*, 1992, **504**, 384 (*synth*)
Sato, A. *et al.*, *Annu. Rep. Sankyo Res. Lab.*, 1995, **47**, 1-58 (*N-Tetradecanoylholothin*)
Li, J. *et al.*, *J. Nat. Prod.*, 1995, **58**, 1081-1086 (*N-Butanoylpyrrothine, N-3-Methylbutanoylpyrrothine*)
Lamari, L. *et al.*, *J. Antibiot.*, 2002, **55**, 696-701; 702-706 (*Saccharothrix pyrrothines*)
Hjelmgaard, T. *et al.*, *Org. Biomol. Chem.*, 2007, **5**, 344-348 (*synth*)

2-(12-Amino-3,7,9-dodecatrienyl)pyridine A-760

12-(2-Pyridinyl)-3,5,9-dodecatrien-1-amine

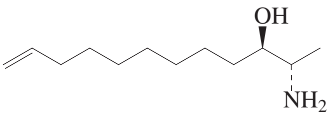


$C_{17}H_{24}N_2$ 256.39

(all-E)-form
Naloamine
[179118-58-2]
Alkaloid from the mollusc *Smaragdinella calyculata*. Amorph. solid. λ_{max} 206 (ϵ 12000); 230 (ϵ 15000); 262 (ϵ 4300); 268 (ϵ 4200); 280 (ϵ 2700) (MeOH).

Szabo, C.M. *et al., Tetrahedron*, 1996, **52**, 9681 (*isol, uv, pmr, cmr, ms, struct*)

2-Amino-11-dodecen-3-ol A-761



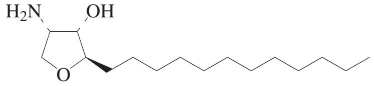
$C_{12}H_{25}NO$ 199.336

(2S,3R)-form
Halaminol B
[389125-59-1]
Isol. from a marine sponge *Haliclona* n. sp. Oil. $[\alpha]_D$ +2.1 (c, 0.06 in CH_2Cl_2).

Clark, R.J. *et al., J. Nat. Prod.*, 2001, **64**, 1568-1571 (*Halaminol B, isol, pmr, cmr*)

4-Amino-2-dodecyltetrahydro-3-furanol A-762

4-Amino-2-dodecyl-3-hydroxytetrahydrofuran

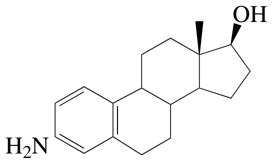


$C_{16}H_{33}NO_2$ 271.442

(2R*,3S*,4S*)-form
N-*(2R-Hydroxyheptadecanoyl):* ***Suillumide***
[1067910-08-0]
$C_{33}H_{65}NO_4$ 539.881
Isol. from *Suillus luteus*. Amorph. solid. $[\alpha]_D^{25}$ +16.3 (c, 0.1 in $CHCl_3$).

León, F. *et al., Chem. Biodiversity*, 2008, **5**, 120-125 (*isol, pmr, cmr, ms*)

3-Aminoestra-1,3,5(10)-trien-17-ol A-763



$C_{18}H_{25}NO$ 271.402

17β-form
Hedonegamin
[10427-24-4]
Constit. of the female of fossil plant *Palaeogelos doleros*. Cryst. (EtOAc). Mp 144-146° (63-65°).

Dannenberg, H. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1967, **348**, 775-782 (*synth*)
Roedder, W. *et al., Pharm. Ztg.*, 1976, **121**, 479-484 (*isol*)
Smith, W.B. *et al., Org. Prep. Proced. Int.*, 1990, **22**, 501-506 (*synth, cmr*)

2-Aminoethanesulfinic acid, 9CI A-764

Hypotaurine. *Cystaminesulfinic acid*
[300-84-5]
$H_2NCH_2CH_2SO_2H$
$C_2H_7NO_2S$ 109.149
Constit. of rat brain. Found in the marine vestimentiferan worm *Riftia pachyptila* and other marine invertebrates. Mp 186-188°. pK_{a1} 2.16; pK_{a2} 9.56.

Chatagner, F. *et al., C. R. Hebd. Seances Acad. Sci.*, 1951, **232**, 448 (*isol*)
Biochem. Prep., 1963, **10**, 72-75 (*synth*)
Hope, D.B. *et al., J.C.S.(C)*, 1970, 270 (*synth*)
Fellman, J.H. *et al., J. Labelled Compd. Radiopharm.*, 1981, **18**, 765 (*synth*)
Stipanuk, M.H. *et al., Methods Enzymol.*, 1987, **143**, 155 (*hplc*)
Fugler-Domenico, L. *et al., Biol. Amines*, 1989, **6**, 289 (*conformn*)
Chaimbault, P. *et al., Anal. Biochem.*, 2004, **332**, 215-225 (*marine, occur*)

2-Aminoethanesulfonic acid, 9CI A-765

Taurine, 8CI, INN. *Aminoethylsulfonic acid. Ethylaminesulfonic acid. FEMA 3813*
[107-35-7]
$H_2NCH_2CH_2SO_3H$
$C_2H_7NO_3S$ 125.148
Occurs free in animal tissues, bacteria, sponges, red algae, e.g. isol. from *Macrocallista nimbosa*, *Turbo stenogyrus*, *Calyx nicaeensis*, *Geodia gigas*, *Mytilus edulis*. Also from green algae, e.g. *Caulerpa okamurai*, *Caulerpa racemosa*, *Chlorodesmis comosa*, *Codium adherens*, *Codium fragile* and *Enteromorpha linza*. Isol. from marine vestimentarian worm *Riftia pachyptila* and from higher plants, e.g. leguminous seedlings. A non-essential amino acid. Intermed. in metab. of cysteine. Used as an adjunct in treatment of hypercholesterolaemia. Metabolic regulator. Monoclinic prismatic rods with sharp taste. Sol. H_2O, insol. EtOH. Mp 328° (320-325° dec.). pK_{a1} 1.5; pK_{a2} 8.74. Dec. at 300°.

▶ LD_{50} (mus, scu) 6000 mg/kg. WX0175000

Amide: [4378-70-5]
$C_2H_8N_2O_2S$ 124.163
Plates (EtOH) (as hydrochloride). Mp 133° (hydrochloride).

N-*Me:* [107-68-6]
$C_3H_9NO_3S$ 139.175
Widely distributed in marine algae including the red alga *Ptilota pectinata* and green alga *Chlorodesmis comosa*. Also found in sponges *Calyx nereis* and *Halichondria* sp. Prisms. V. sol. H_2O; insol. EtOH, Et_2O. Mp 241-242°.

N,N-*Di-Me:* [637-95-6]
$C_4H_{11}NO_3S$ 153.202
Obt. from *Corallina officinalis*. Present in *Furcellaria fastigiata* and other red algae. Prisms (MeOH). V. sol. H_2O, AcOH, insol. EtOH, Et_2O. Mp 315-316° dec.

N,N-*Bis(2-chloroethyl): Taumustine*
[98277-87-3]
$C_6H_{13}Cl_2NO_3S$ 250.145
Cryst. (H_2O). Mp 178-180°.

N-*(2,3-Dihydroxypropyl):* N-*Glyceryltaurine*
[65222-42-6]
$C_5H_{13}NO_5S$ 199.227
Isol. from the red alga *Gigartina leptorhynchos*. Cryst. (EtOH aq.). Mp 163-164°. $[\alpha]_D^{23}$ -21 (H_2O).

N-*(15-Methyl-9Z-hexadecenoyl):* ***N-(15-Methyl-9-hexadecenoyl)taurine***
[679834-30-1]
$C_{19}H_{37}NO_4S$ 375.572
Isol. from the sponge *Erylus nobilis*.

N-*(5Z,8Z,11Z,14Z-Eicosatetraenoyl):* N-*(5,8,11,14-Eicosatetraenoyl)taurine*
[679834-28-7]
$C_{22}H_{37}NO_4S$ 411.605
Isol. from the starfish *Certonardoa semiregularis*.

[7347-25-3 , 4316-74-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 890A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1433C (*nmr*)
Org. Synth., Coll. Vol., 2, 1943, 563; 564 (*synth*)
Ishidate, M. *et al., Chem. Pharm. Bull.*, 1954, **2**, 275-279 (*synth*)
Lindberg, B. *et al., Acta Chem. Scand.*, 1955, **9**, 1093-1096; 1323-1326 (*isol, N-Me, N,N-di-Me*)
Wickberg, B. *et al., Acta Chem. Scand.*, 1956, **10**, 1097-1099 (*Glyceryltaurine*)
Sutherland, H.H. *et al., Acta Cryst.*, 1963, **16**, 897-901 (*cryst struct*)
Huxtable, R. *et al., Taurine, [Int. Symp.], 1st, 1975 (1976)*, (Eds.), Raven Press, New York, 1975, (*book*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1984, 124-125; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 126-127 (*N-Me, occur*)
Hashem, K.M.E. *et al., Bull. Soc. Chim. Belg.*, 1985, **94**, 735-754 (*cmr*)
Taurine: Nutritional Value and Mechanisms of Action, (eds. Lombardini, J.B. *et al*), Plenum Press, 1992, (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1419
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1665-1666 (*use, occur*)
Merck Index, 13th edn., 2001, No. 9163 (*bibl*)
Hibbs, D.E. *et al., Chem. Eur. J.*, 2003, **9**, 1075-1084 (*cryst struct*)
Wang, W. *et al., Nat. Prod. Sci.*, 2003, **9**, 241-244; *CA*, **140**, 335912 (*N-Methylhexadecenoyl, N-Eicosatetraenoyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TAG750

2-Aminoethanesulfonothioic acid, 9CI A-766

S-*(2-Aminoethyl) thiosulfate, 8CI.* ***Thiotaurine***
[2937-54-4]
[31999-89-0 (Na salt)]

$H_2NCH_2CH_2SO_2SH$

$C_2H_7NO_2S_2$ 141.215

Isol. from various marine invertebrates incl. *Bathymodiolus* spp., *Calyptogena magnifica* and *Riftia pachyptila*. Biomarker of sulfur-based symbiosis in deep-sea bivalves. Cryst. (EtOH aq.). Mp 213° dec.

Sörbö, B.H. *et al., Acta Chem. Scand.*, 1958, **12**, 146 (*synth*)
Biochem. Prep., 1963, **10**, 72-75 (*synth*)
Pruski, A.M. *et al., J. Exp. Biol.*, 2003, **206**, 2923-2930 (*biosynth*)
Chaimbault, P. *et al., Anal. Biochem.*, 2004, **332**, 215-225 (*occur*)

2-Aminoethanol, 9CI A-767

2-Hydroxyethylamine. Ethanolamine. Monoethanolamine. Colamine. Olamine

[141-43-5]

$H_2NCH_2CH_2OH$

C_2H_7NO 61.083

Manuf. from ethylene oxide and NH_3. Widely distributed in biol. tissues. Component of lecithin. Constit. of defence secretions of *Chrysolina* and related beetles. Chemical intermed., org. base. Removes CO_2 and H_2S from gases. Reagent for fluorimetric anal. of carbohydrates by hplc. Selectively cleaves the glycosyl ester bond of peracylated aldoses. Curing agent for epoxy resins. Viscous, hygroscopic liq. Misc. H_2O, MeOH, Me_2CO; spar. sol. C_6H_6, Et_2O. d_4^{25} 1.01. Mp 10.5°. Bp 171°. n_D^{20} 1.4539. pK_a 9.47. Vp 0.48 mmHg (20°).

▶ Fl. p. 85°, autoignition temp. 410°. Corrosive and irritating to skin, eyes and mucous membranes. LD_{50} (rat, orl) 1720 mg/kg. Exp. teratogen. OES: long-term 3 ppm; short-term 6 ppm. KJ5775000

O-*Ac:* **O-*Acetylethanolamine***. *2-Acetoxyethylamine*
[1854-30-4]
$C_4H_9NO_2$ 103.121
Isol. from seeds of *Lens culinaris* (lentil), also present in other Fabaceae. Shows antiinflammatory props., stimulates cockroach heart. $Bp_{0.3}$ 134-135°.

N-*(9*Z*,12*Z*-Octadecadienoyl):* N-*(2-Hydroxyethyl)-9,12-octadecadienamide, 9CI*. **N-*(2-Hydroxyethyl)linoleamide***
[68171-52-8]
[10015-67-5]
$C_{20}H_{37}NO_2$ 323.518
Alkaloid from *Vaccaria segetalis*.

[96-80-0 , 20739-39-3]

Hayman, A.R. *et al., Phytochemistry*, 1987, **26**, 839 (*O-Acetylethanolamine*)
Sang, S. *et al., CA*, 1999, **130**, 349718n (*N-Hydroxyethyllinoleamide, isol*)

2-Aminoethyl dihydrogen phosphate A-768

Ethanolamine O-*phosphate*. O-*Phosphoethanolamine*

[1071-23-4]

$H_2NCH_2CH_2OP(O)(OH)_2$

$C_2H_8NO_4P$ 141.063

Isol. from eye lens tissue and gram-negative bacteria. Intermed. in phosphoglyceride biosynth. in mammals. Cryst. (EtOH aq.). Mp 242° (231.5-234°).

Mono-Et ester: Ethyl hydrogen 2-aminoethyl phosphate
$C_4H_{12}NO_4P$ 169.117
Cryst. (EtOH/Me_2CO). Mp 238°.

Diisopropyl ester: Diisopropyl 2-aminoethyl phosphate
[14646-04-9]
$C_8H_{20}NO_4P$ 225.224
Liq. $Bp_{0.06}$ 75°.

Mono-Ph ester: Phenyl hydrogen 2-aminoethyl phosphate
$C_8H_{12}NO_4P$ 217.161
Solid. V. sol. H_2O; spar. sol. EtOH; insol. C_6H_6, $CHCl_3$, Et_2O.

N-*Ac: 2-Acetamidoethyl phosphate*
[89603-45-2]
$C_4H_{10}NO_5P$ 183.101
Occurs in O-antigen polysaccharide of *Proteus mirabilis* 038. No phys. props. reported.

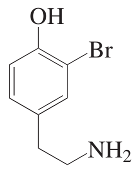
[87111-65-7 , 3724-89-8 , 18672-70-3 , 19077-76-0 , 131703-98-5 , 61020-38-0 , 31512-55-7 , 32607-10-6 , 37785-54-9 , 63441-18-9]

Plapinger, R.E. *et al., J.A.C.S.*, 1953, **75**, 5757
Cherbuliez, E. *et al., Helv. Chim. Acta*, 1956, **39**, 1455-1461 (*N-Ac, synth*)
Tsizin, Y.S. *et al., Zh. Obshch. Khim.*, 1963, **33**, 2873; *J. Gen. Chem. USSR (Engl. Transl.)*, 1963, **33**, 2800 (*synth, ir*)
Greenhalgh, R. *et al., Can. J. Chem.*, 1967, **45**, 495 (*diisopropyl ester, synth, ir, pmr, P nmr*)
Greiner, J.V. *et al., Exp. Eye Res.*, 1982, **34**, 545 (*P-31 nmr*)
Glonek, T. *et al., J. Neurochem.*, 1982, **39**, 1210 (*P-31 nmr*)
Trigalo, F. *et al., J.C.S. Perkin 1*, 1982, 1733 (*monoethyl ester*)
Weber, H.P. *et al., Acta Cryst. B*, 1984, **40**, 506 (*cryst struct*)
Cates, L.A. *et al., J. Med. Chem.*, 1984, **27**, 654 (*synth*)
Hayase, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2251 (*isol, ir, pmr, cmr*)
Bissinger, P. *et al., Chem. Ber.*, 1991, **124**, 509 (*synth, salts, cryst struct*)
Ger. Pat., 1993, 4 141 842; *CA*, **120**, 57142 (*N-Ac, synth*)
Kandakova, A.N. *et al., Carbohydr. Res.*, 2003, **338**, 2387-2392 (*N-Ac, occur*)

4-(2-Aminoethyl)-2-bromophenol, 9CI A-769

2-(3-Bromo-4-hydroxyphenyl)ethylamine. 3-Bromotyramine

[104616-74-2]



$C_8H_{10}BrNO$ 216.077

Isol. from the ascidian *Cnemidocarpa bicornuta*. Cryst. Mp 162-164°. λ_{max} 203 (log ε 4.4); 283 (log ε 3.3) (MeOH).

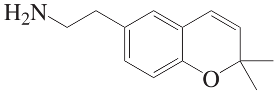
Hydrochloride:
Cryst. (MeOH/EtOAc). Mp 205.5-207°.

N,N,N-*Tri-Me: 3-Bromo-4-hydroxy-*N,N,N-*trimethylbenzeneethanaminium, 9CI. 3-Bromo-*N,N,N-*trimethyltyramine*
[259533-84-1]
$C_{11}H_{17}BrNO^{\oplus}$ 259.165
Isol. from the sponge *Verongula gigantea*. Isol. as trifluoroacetate salt. λ_{max} 281 (ε 1485) (MeOH).

Tolkachev, O.N. *et al., Zh. Obshch. Khim.*, 1958, **28**, 3320-3323; *J. Gen. Chem. USSR (Engl. Transl.)*, 1958, **28**, 3345-3348 (*synth*)
Lindsay, B.S. *et al., J. Nat. Prod.*, 1998, **61**, 857-858 (*isol, uv, ir, pmr, cmr, ms*)
Ciminiello, P. *et al., J. Nat. Prod.*, 2000, **63**, 263-266 (*N-tri-Me deriv*)

6-(2-Aminoethyl)-2,2-dimethyl-2*H*-1-benzopyran A-770

*(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)ethanamine*



$C_{13}H_{17}NO$ 203.283

N-*(2-Methylpropanoyl):* [124704-80-9]
$C_{17}H_{23}NO_2$ 273.374
Alkaloid from roots of *Amyris sylvatica* (Rutaceae).

N-*(3-Methylbutanoyl):* [124704-79-6]
$C_{18}H_{25}NO_2$ 287.401
Alkaloid from roots of *Amyris sylvatica* (Rutaceae). Mp 104-105°.

N-*Benzoyl:* N-*[2-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)ethyl]benzamide, 9CI*. ***6-(2-Benzamidoethyl)-2,2-dimethyl-2*H*-1-benzopyran***
[89764-18-1]
$C_{20}H_{21}NO_2$ 307.391
Alkaloid from the aerial portions of *Amyris plumieri* (Rutaceae). Mp 133.5-134.5°.

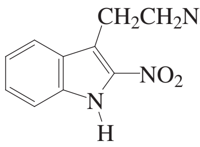
N-*(3-Pyridinecarbonyl):* **N-*[2-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)ethyl]-3-pyridinecarboxamide, 9CI***
[69142-83-2]
$C_{19}H_{20}N_2O_2$ 308.379
Alkaloid from *Amyris plumieri* (Rutaceae). Mp 99-100°.

N-*(3-Pyridinecarbonyl),* N-*Me:* **N-*[2-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)ethyl]*-N-*methyl-3-pyridinecarboxamide***
[137132-29-7]
$C_{20}H_{22}N_2O_2$ 322.406
Alkaloid from *Amyris texana* (Rutaceae). Oil.

Burke, B.A. *et al., Tet. Lett.*, 1978, **19**, 2723-2726 (*N-3-pyridinecarbonyl*)
Philip, S. *et al., Heterocycles*, 1984, **22**, 9-12 (*N-benzoyl*)
Hasbun, C. *et al., J. Nat. Prod.*, 1989, **52**, 868-870 (*Amyris sylvatica constit*)
De la Fuente, G. *et al., Phytochemistry*, 1991, **30**, 2677-2684 (*Amyris texana constit*)

3-(2-Aminoethyl)-2-nitroindole A-771

*2-Nitro-1*H*-indole-3-ethanamine. 2-Nitrotryptamine*



$C_{10}H_{11}N_3O_2$ 205.216

N^b*-Ac:* **N^b*-Acetyl-2-nitrotryptamine***
$C_{12}H_{13}N_3O_3$ 247.253
Isol. from the marine-derived *Flavobacterium* sp. T436.

Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*Ac, isol*)

(2-Aminoethyl)phosphinic acid, 9CI A-772

(2-Aminoethyl)phosphonous acid. 2-(Hydroxyphosphinyl)ethylamine. Antibiotic MP 105. MP 105
[85618-16-2]
$H_2NCH_2CH_2PH(O)OH \Leftrightarrow H_2NCH_2CH_2P(OH)_2$

$C_2H_8NO_2P$ 109.064
Prod. by *Streptomyces hygroscopicus* SF-1293. Amorph. powder. Mp 208-210° dec. (natural) Mp 255° (synthetic).

Seto, H. *et al., Biochem. Biophys. Res. Commun.*, 1983, **111**, 1008-1014 (*isol*)
Dingwall, J.G. *et al., Tetrahedron*, 1989, **45**, 3787-3808 (*synth, pmr, P-31 nmr*)
Berlicki, L. *et al., J.O.C.*, 2005, **70**, 6340-6349 (*synth*)

(2-Aminoethyl)phosphonic acid, 9CI A-773

Ciliatine. *AEP*
[2041-14-7]
$H_2NCH_2CH_2P(O)(OH)_2$

$C_2H_8NO_3P$ 125.064
Constit. as glyceryl esters of rumen protozoan, *Tetrahymena pyriformis*, sea anemones, bovine brain, mycobacteria, and a fungus *Pythium prolatum*. Rhombic cryst. or needles (EtOH aq.). Mp 295-297° dec. pK_{a1} 2.45; pK_{a2} 7; pK_{a3} 10.8. pK_{a1} 1.3; pK_{a2} 6.51; pK_{a3} 11.5 (25°). The metastable rhombic form is difficult to prepare. First known natural compd. contg. the C–P bond.

Di-Et ester: [41468-36-4]
$C_6H_{16}NO_3P$ 181.171
Liq. $Bp_{0.025}$ 54-56°.

N*-Benzoyl: 2-(Benzoylamino)ethylphosphonic acid*
$C_9H_{12}NO_4P$ 229.172
Solid. Mp 191-192°.

N*-Me:* N*-Methylciliatine. 2-(Methylamino)ethylphosphonic acid*
[14596-55-5]
$C_3H_{10}NO_3P$ 139.091
Isol. from the sea anemone *Anthopleura xanthogrammica*. Needles (MeOH aq.). Mp 291° dec.

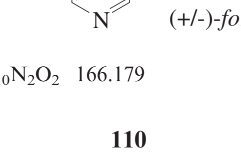
N,N*-Di-Me: 2-Dimethylaminoethylphosphonic acid.* N,N*-Dimethylciliatine*
[14596-56-6]
$C_4H_{12}NO_3P$ 153.117
Isol. from *Anthopleura xanthogrammica*. Pale yellow cryst. (MeOH aq.). Mp 249.5° dec.

N,N*-Di-Me, Et ester:* [41948-36-1]
$C_6H_{16}NO_3P$ 181.171
Bp_1 100°.

N*-Phthalimide, di-Et ester: Diethyl (2-phthalimidoethyl)phosphonate*
$C_{14}H_{18}NO_5P$ 311.274
Cryst. (Et_2O/petrol). Mp 58°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1477A (*nmr*)
Kosolapoff, G.M. *et al., J.A.C.S.*, 1947, **69**, 2112 (*synth*)
Top. Phosphorus Chem., Interscience, 1966, **4**, 23: **11**; 297 (*rev*)
Barycki, J. *et al., Tet. Lett.*, 1970, 3147 (*synth*)
Isbell, A.F. *et al., J.O.C.*, 1972, **37**, 4399 (*synth, bibl*)
Harvey, D.J. *et al., J. Chromatogr.*, 1973, **79**, 65 (*ms*)
Lagrange, C.G. *et al., Can. J. Chem.*, 1978, **56**, 663 (*ir, Raman*)
Brigot, D. *et al., Tetrahedron*, 1979, **35**, 1345 (*synth, pmr, derivs*)
Fabre, G. *et al., Can. J. Chem.*, 1981, **59**, 2864 (*synth, di-Et ester, ir, pmr*)
Varlet, J.M. *et al., Tetrahedron*, 1981, **37**, 3713 (*dervis*)
Al-Rawi, J.M.A. *et al., Org. Magn. Reson.*, 1983, **21**, 75 (*di-Et ester, cmr*)
Appleton, T.G. *et al., Aust. J. Chem.*, 1984, **37**, 1833 (*props, cmr, P-31 nmr*)
Yamauchi, K. *et al., J.O.C.*, 1984, **49**, 1158 (*N-phthalimide deriv*)
Gubnitskaya, E.S. *et al., Zh. Obshch. Khim.*, 1986, **56**, 2017; *J. Gen. Chem. USSR (Engl. Transl.)*, 1986, **56**, 1779 (*esters, synth, ir*)
Osapay, G. *et al., Tetrahedron*, 1987, **43**, 2977 (*ir, pmr*)
Lazukina, L.A. *et al., Zh. Obshch. Khim.*, 1988, **58**, 939; *J. Gen. Chem. USSR (Engl. Transl.)*, 1988, **58**, 833 (*synth, P-31 nmr*)
Thayer, J.S. *et al., Appl. Organomet. Chem.*, 1989, **3**, 203 (*rev*)
Warielewski, C. *et al., J. Prakt. Chem.*, 1989, **331**, 507 (*synth, ir*)
Harris, R.K. *et al., Magn. Reson. Chem.*, 1989, **27**, 470 (*cmr, N-15 nmr, P-31 nmr*)
Glowacki, Z. *et al., Magn. Reson. Chem.*, 1989, **27**, 897 (*cmr*)
Warielewski, C. *et al., Synthesis*, 1989, 52 (*synth, ir, pmr*)
Ohashi, K. *et al., Tetrahedron*, 1989, **45**, 2557 (*N-Me, synth, ir*)
Hayashi, A. *et al., Chem. Phys. Lipids*, 1990, **52**, 57 (*fab-ms*)
Neidlein, R. *et al., Helv. Chim. Acta*, 1992, **75**, 2545 (*N-phthalimide deriv*)
Ohno, K. *et al., J. Mol. Struct.*, 1993, **298**, 1 (*ir, Raman, conformn*)
Fields, S.C. *et al., Tetrahedron*, 1999, **55**, 12237-12273 (*rev, synth*)

5-(1-Aminoethyl)-3-pyridinecarboxylic acid, 9CI A-774



(+/-)-*form*

$C_8H_{10}N_2O_2$ 166.179

(±)-*form*

Me ester:
Syrup.

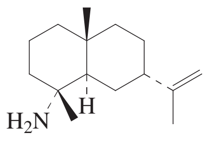
p*-Nitrobenzoyl:*
Needles. Mp 154-157°.

(ξ)-*form*

Me ester: ***Methyl 5-(1-aminoethyl)-3-pyridinecarboxylate, 9CI***. *3-(1-Aminoethyl)-5-carbomethoxypyridine*
[38940-68-0]
$C_9H_{12}N_2O_2$ 180.206
Alkaloid from *Nauclea diderrichii* (Rubiaceae). Oil. $[\alpha]_D^{25}$ +27 (c, 0.34 in MeOH).

McLean, S. *et al., Can. J. Chem.*, 1971, **50**, 1478 (*isol, ms, pmr, uv, synth*)

4-Amino-11-eudesmene A-775



$C_{15}H_{27}N$ 221.385

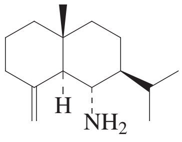
(4α,7α)-*form* [442851-12-9]
[442851-11-8]
Constit. of *Axinyssa ambrosia*. Oil; cryst. (as hydrochloride). Mp 210-220° (hydrochloride). $[\alpha]_D$ -17.5 (c, 0.9 in $CHCl_3$).

N*-Formyl:* ***4-Formamido-11-eudesmene***
[442851-14-1]
$C_{16}H_{27}NO$ 249.395
Constit. of *Axinyssa ambrosia*. Cryst. Mp 104-107°. $[\alpha]_D$ -10 (c, 0.22 in $CHCl_3$).

4-Isocyanide: ***4-Isocyano-11-eudesmene***
[442851-13-0]
$C_{16}H_{25}N$ 231.38
Constit. of *Axinyssa ambrosia*. Oil. $[\alpha]_D$ -15 (c, 0.2 in $CHCl_3$). Has -NC in place of NH_2.

Petrichtcheva, N.V. *et al., J. Nat. Prod.*, 2002, **65**, 851-855 (*isol, pmr, cmr*)

6-Amino-4(15)-eudesmene A-776



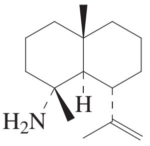
$C_{15}H_{27}N$ 221.385

6α-*form*
Halichonadin D
[847605-79-2]
Constit. of a *Halichondria* sp. Yellow oil. $[\alpha]_D^{27}$ +18 (c, 0.2 in $CHCl_3$).

N*-Methoxycarbonyl:* ***Halichonadin B***
[847605-77-0]
$C_{17}H_{29}NO_2$ 279.422
Constit. of a *Halichondria* sp. Amorph. solid. $[\alpha]_D^{24}$ -10 (c, 1 in $CHCl_3$).

Ishiyama, H. *et al.*, *Tetrahedron*, 2005, **61**, 1101-1105 (*isol, pmr, cmr*)

4-Amino-11-gorgonene A-777



$C_{15}H_{27}N$ 221.385

(4α,6α)-*form*

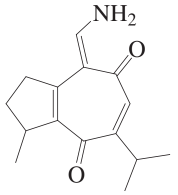
N-*Formyl: 4-Formamido-11-gorgonene*
[134781-19-4]
$C_{16}H_{27}NO$ 249.395
Isol. from the molluscs *Phyllidia pustulosa* and *Phyllidia varicosa*. Cryst. [α]$_D$ -61.8 (c, 0.11 in $CHCl_3$). Mp >300° dec.

4-Isocyanide: ***4-Isocyano-11-gorgonene***
[134781-18-3]
$C_{16}H_{25}N$ 231.38
Isol. from the molluscs *Phyllidia pustulosa* and *Phyllidia varicosa*. Oil. [α]$_D$ -66.9 (c, 1.6 in $CHCl_3$).

4-Isothiocyanate: 4-Isothiocyanato-11-gorgonene
[134781-20-7]
$C_{16}H_{25}NS$ 263.446
Isol. from *Phyllidia pustulosa*. Oil. [α]$_D$ -101.6 (c, 0.5 in $CHCl_3$).

Kassühlke, K.E. *et al.*, *J.O.C.*, 1991, **56**, 3747-3750 (*isol, pmr, cmr, ms*)

14-Amino-1(5),7,10(14)-guaiatriene-6,9-dione A-778



$C_{15}H_{19}NO_2$ 245.321

(4ξ,10*Z*)-*form*
Muscicapine A
[873684-18-5]
Alkaloid from the roots of *Croton muscicapa*. Amorph. yellow solid. [α]$_D^{20}$ -44 (c, 0.05 in $CHCl_3$).

N-*(2-Methylbutyl):* ***Muscicapine C***
[873684-20-9]
$C_{20}H_{29}NO_2$ 315.455
Alkaloid from the roots of *Croton muscicapa*. Yellow oil. [α]$_D^{20}$ -9 (c, 0.05 in $CHCl_3$).

N-*(3-Methylbutyl):* ***Muscicapine B***
[873684-19-6]
$C_{20}H_{29}NO_2$ 315.455
Alkaloid from the roots of *Croton muscicapa*. Yellow oil. [α]$_D^{20}$ -6 (c, 0.02 in $CHCl_3$).

Araújo-Júnior, V.T. *et al.*, *J. Braz. Chem. Soc.*, 2005, **16**, 553-557 (*isol, pmr, cmr, ms*)

3-Amino-5-guanidinopentanoic acid A-779

3-Amino-5-[(aminoiminomethyl)amino]-pentanoic acid, 9CI. β-Arginine
$HN{=}C(NH_2)NHCH_2CH_2$-
$CH(NH_2)CH_2COOH$

$C_6H_{14}N_4O_2$ 174.202

N^3-*Me: 5-[(Aminoiminomethyl)amino]-3-(methylamino)pentanoic acid, 9CI. 5-Guanidino-3-methylaminopentanoic acid*
[67396-07-0]
$C_7H_{16}N_4O_2$ 188.229
Component of Antibiotic LL-BM 547β.

McGahren, W.J. *et al.*, *J.O.C.*, 1977, **42**, 1282
Nomoto, S. *et al.*, *Chem. Lett.*, 1978, 589 (*synth*)

1-Amino-20-guanidino-4,8,12,16-tetraazaicosane A-780

22-Amino-2,7,11,15,19-pentaazadocosanimidamide
[864812-20-4]
$H_2N(CH_2)_3NH(CH_2)_3NH(CH_2)_3NH(CH_2)_3NH(CH_2)_4NHC(^{\omega}NH_2){=}NH$

$C_{17}H_{42}N_8$ 358.572
Isol. from the venom of the spider *Paracoelotes birulai.*

N$^{\omega}$-*Ac:* [864812-18-0]
$C_{19}H_{44}N_8O$ 400.61
Isol. from the venom of *Paracoelotes birulai.*

Tzouros, M. *et al.*, *Toxicon*, 2005, **46**, 350-354

1-Amino-16-guanidino-4,8,12-triazahexadecane A-781

18-Amino-2,7,11,15-tetraazaoctadecanimidamide, 9CI
[864812-13-5]
$H_2N^1(CH_2)_3^4NH(CH_2)_3NH(CH_2)_3NH(CH_2)_4NHC(NH_2){=}NH$

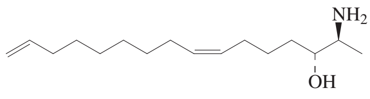
$C_{14}H_{35}N_7$ 301.477
Isol. from the venom of the spider *Paracoelotes birulai.*

N^1-*Ac:* [864812-15-7]
$C_{16}H_{37}N_7O$ 343.515
Isol. from the venom of the spider *Paracoelotes birulai.*

*4-*N-*Hydroxy:* [864812-14-6]
$C_{14}H_{35}N_7O$ 317.477
Isol. from the venom of the spider *Paracoelotes birulai.*

Tzouros, M. *et al.*, *Toxicon*, 2005, **46**, 350-354 (*isol, 4-N-hydroxy, N^1-Ac*)

2-Amino-7,15-hexadecadien-3-ol A-782

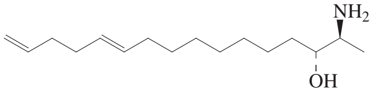


$C_{16}H_{31}NO$ 253.427

(2*S*,3*R*,7*Z*)-*form*
Obscuraminol B
[350485-82-4]
Isol. from the tunicate *Pseudodistoma obscurum*. Oil (as di-Ac). [α]$_D^{24}$ -21.1 (c, 0.65 in MeOH) (di-Ac).

Garrido, L. *et al.*, *Tetrahedron*, 2001, **57**, 4579-4588 (*isol, pmr, cmr, abs config*)

2-Amino-11,15-hexadecadien-3-ol A-783



$C_{16}H_{31}NO$ 253.427

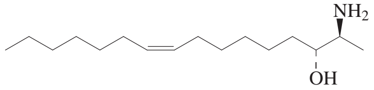
(2*S*,3*R*,11*E*)-*form*
Obscuraminol C
[350484-95-6]
Isol. from the tunicate *Pseudodistoma obscurum*. Amorph. solid (as di-Ac). [α]$_D^{24}$ -24.5 (c, 0.83 in MeOH) (di-Ac).

11,12-Dihydro: 2-Amino-15-hexadecen-3-ol. ***Obscuraminol F***
[350485-01-7]
$C_{16}H_{33}NO$ 255.443
Isol. from *Pseudodistoma obscurum*. Amorph. solid (as di-Ac). [α]$_D^{24}$ -19.2 (c, 0.71 in MeOH) (di-Ac).

15,16-Dihydro: 2-Amino-11-hexadecen-3-ol. ***Obscuraminol E***
[350485-00-6]
$C_{16}H_{33}NO$ 255.443
Isol. from *Pseudodistoma obscurum*. Oil (as di-Ac).

Garrido, L. *et al.*, *Tetrahedron*, 2001, **57**, 4579-4588 (*Obscuraminols C,E,F, isol, pmr, cmr, abs config*)

2-Amino-9-hexadecen-3-ol A-784



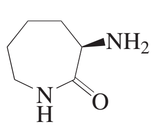
$C_{16}H_{33}NO$ 255.443

(2*S*,3*R*,9*Z*)-*form*
Obscuraminol D
[350484-99-0]
Isol. from the tunicate *Pseudodistoma obscurum*. Oil (as di-Ac). [α]$_D^{24}$ -21.6 (c, 0.44 in MeOH) (di-Ac).

Garrido, L. *et al.*, *Tetrahedron*, 2001, **57**, 4579-4588 (*isol, ir, pmr, cmr, abs config*)

3-Aminohexahydro-2*H*-azepin-2-one, 9CI A-785

3-Amino-ϵ-caprolactam
[671-42-1]



(*R*)-*form*

$C_6H_{12}N_2O$ 128.174

(*R*)-*form* [28957-33-7]

Hydrochloride: [26081-03-8]
Solid (MeOH). [α]$_D^{26}$ +26.4 (c, 4 in 1*M* HCl) (>99% ee).

Hydrobromide: [16473-63-5]
$[\alpha]_D^{20}$ +20.7 (c, 5 in H_2O).

(S)-form [21568-87-6]
Mp 71-72°. $[\alpha]_D^{25}$ -34 (c, 4 in 1*M* HCl) (100% ee).

Hydrochloride: [26081-07-2]
Mp 270°. $[\alpha]_D^{25}$ -27 (c, 2.98 in 1*M* HCl).

Hydrobromide: [16473-62-4]
Mp 285-288° dec. $[\alpha]_D^{20}$ -20.7 (c, 5 in H_2O).

N^3-*(6-Methyloctanoyl):* ***Caprolactin B***
[151379-42-9]
$C_{15}H_{28}N_2O_2$ 268.398
Isol. from a marine bacterium. Cytotoxic agent. $[\alpha]_D^{22}$ +5.4 (c, 1.03 in CH_2Cl_2). Isol. as a mixt. with Caprolactin A. Data given is for the mixt. λ_{max} 219 ; 274 (sh) (MeOH).

N^3-*(7-Methyloctanoyl):* ***Caprolactin A***
[151379-41-8]
$C_{15}H_{28}N_2O_2$ 268.398
Isol. from a marine bacterium. Cytotoxic agent. Isol. as a mixt. with Caprolactin B. λ_{max} 219 ; 274 (MeOH) (Berdy).

(±)-*form* [17929-90-7]
Cryst. (EtOAc). Mp 68-71° Mp 147-149°. $Bp_{0.1}$ 105°.

Hydrochloride: [29426-64-0]
Mp 294-296°.

Picrate:
Needles (H_2O). Mp 233° dec.

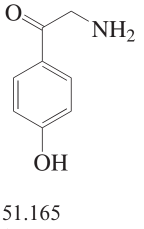
N-*Ac:*
$C_8H_{14}N_2O_2$ 170.211
Cryst. (EtOAc). Mp 160-162°.

N-*Benzoyl:*
$C_{13}H_{16}N_2O_2$ 232.282
Cryst. (EtOH). Mp 203-211°.

Pellegata, R. *et al., Synthesis*, 1978, 614 (*synth, S-form*)
Boyle, W.J. *et al., J.O.C.*, 1979, **44**, 4841 (*synth*)
Davidson, B.S. *et al., Tetrahedron*, 1993, **49**, 6569-6574 (*Caprolactins*)
Uchikawa, J. *et al., J. Het. Chem.*, 1994, **31**, 877 (*N-Ac, N-benzoyl*)
Sakai, K. *et al., Tetrahedron: Asymmetry*, 2003, **14**, 3713-3718 (***resoln***)
Urbanczyk-Lipkowska, Z. *et al., Tetrahedron: Asymmetry*, 2007, **18**, 1254-1256 (*resoln, S-form*)

2-Amino-4′-hydroxyacetophenone A-786

2-Amino-1-(4-hydroxyphenyl)ethanone, 9CI. p-*Hydroxyphenacylamine*
[77369-38-1]



$C_8H_9NO_2$ 151.165
Plates (EtOH). Mp 190-193° dec.

Hydrochloride: [19745-72-3]
Needles (HCl aq.), prisms (EtOH). Mp 241-245° Mp 249-251° dec.

N-*(4-hydroxy-3-methoxy-*E*-cinnamoyl):* ***Terrestriamide***
[157536-49-7]
$C_{18}H_{17}NO_5$ 327.336
Alkaloid from the fruit of *Tribulus terrestris*. Light yellow cryst. Mp 218-220°.

N-*Di-Me:*
$C_{10}H_{13}NO_2$ 179.218
Prisms (Et_2O/petrol). Mp 142°.

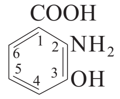
Me ether: 2-Amino-4′-methoxyacetophenone
[3883-94-1]
$C_9H_{11}NO_2$ 165.191 HCl
Cryst. (EtOH) (as hydrochloride). Mp 200-201° (hydrochloride). CAS no. refers to hydrochloride.

[40513-43-7]

Tutin, F. *et al., J.C.S.*, 1910, **97**, 2520
Mannich, C. *et al., Ber.*, 1911, **44**, 1547
Voswinckel, H. *et al., Ber.*, 1912, **45**, 1005
Mannich, C. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1915, **253**, 193
Corrigan, J.R. *et al., J.A.C.S.*, 1945, **67**, 1894
Yinglin, H. *et al., Synthesis*, 1990, 615 (*Me ether, synth, ir, pmr*)
Ren, Y.J. *et al., Yaoxue Xuebao*, 1994, **29**, 204 (*Terrestriamide*)

2-Amino-3-hydroxybenzoic acid A-787

3-Hydroxyanthranilic acid
[548-93-6]



$C_7H_7NO_3$ 153.137
Metab. of Tryptophan, T-640 in humans, rats and *Claviceps* spp. Isol. from cultures of *Klebsiella pneumoniae*. Also isol. from *Brassica oleracea* (cauliflower). Leaflets (H_2O). Mp 164°. pK_{a2} 5.19; pK_{a3} 10.12 (20°).

▶ Exp. carcinogen. DG2625000

Hydrochloride: [4920-81-4]
Cryst. (HCl). Mp 198-200°.

N-*Ac, amide: 2-Acetamido-3-hydroxybenzamide*
$C_9H_{10}N_2O_3$ 194.19
Prod. by *Streptomyces* sp. GW37/3236. Solid. λ_{max} 240 (sh) ; 295 (log ε 3.68) (MeOH).

Me ether: 2-Amino-3-methoxybenzoic acid. 3-Methoxyanthranilic acid
[3177-80-8]
$C_8H_9NO_3$ 167.164
Leaflets (AcOH). Mp 170-171°.

Trifluoromethyl ether:
$C_8H_6F_3NO_3$ 221.136
Needles (H_2O). Mp 99-101°.

O,N-*Di-Me: 3-Methoxy-2-methylaminobenzoic acid. Damascenenic acid. Damascenic acid*
[485-27-8]
$C_9H_{11}NO_3$ 181.191
Mp 144°. Forms a trihydrate, Mp 80°.

O,N-*Di-Me; hydrochloride:* Mp 210-211°.

O,N-*Di-Me, Me ester:* ***Damascenine***
[483-64-7]
$C_{10}H_{13}NO_3$ 195.218
Alkaloid from seeds of *Nigella damascena* (Ranunculaceae). Mp 24-26°. Bp 270° dec. Bp_{10} 147-148°.

O,N-*Di-Me, Me ester; hydrochloride:*
Cryst. + $1H_2O$. Mp 122° Mp 156° (anhyd.).

O,N-*Di-Me, Me ester, picrate:* Mp 158-159°.

Me ether, nitrile: 2-Amino-3-methoxybenzonitrile. 2-Cyano-6-methoxyaniline
[148932-68-7]
$C_8H_8N_2O$ 148.164
Powder. Mp 64-67°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 206C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1098C; 1123C (*nmr*)
CRC Atlas of Spectral Data and Physical Constants, b842 (*uv, ir*)
Ewins, A.J. *et al., J.C.S.*, 1912, **101**, 544-552 (*Damascenine*)
Froelicher, V. *et al., J.C.S.*, 1921, **119**, 1425-1432 (*Me ether, synth*)
Muelle, F. *et al., Planta*, 1961, **57**, 403-477 (*isol*)
Munsche, D. *et al., Phytochemistry*, 1965, **4**, 705-712 (*biosynth*)
Kuhn, R. *et al., Chem. Ber.*, 1968, **101**, 3597-3603 (*Damascenine*)
Kuznezova, L.E. *et al., Nature (London)*, 1969, **222**, 484-485 (*props*)
Thoinet, M. *et al., Ann. Pharm. Fr.*, 1978, **36**, 337-339 (*synth, Damascenine*)
Mohr, N. *et al., Annalen*, 1981, 1515-1518 (*isol*)
Okabe, N. *et al., Acta Cryst. C*, 1996, **52**, 2345-2347 (*cryst struct*)
Goto, K. *et al., Chem. Pharm. Bull.*, 1996, **44**, 547-551 (*Me ether nitrile*)
Nagasaka, T. *et al., J.O.C.*, 1998, **63**, 6797-6801 (*Me ether, synth, ir, pmr*)
Leroux, F. *et al., J.O.C.*, 2003, **68**, 4693-4699 (*trifluoromethyl ether, synth, pmr, cmr*)
Fotso, S. *et al., Z. Naturforsch., B*, 2003, **58**, 1242-1246 (*2-Acetamido-3-hydroxybenzamide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKE750

2-Amino-4-hydroxybenzoic acid A-788

4-Hydroxyanthranilic acid
[38160-63-3]

$C_7H_7NO_3$ 153.137
Needles (H_2O). Mp 148° (dec.).

Hydrochloride:
Needles.

Me ester:
$C_8H_9NO_3$ 167.164
Needles. Mp 132-133°.

Me ether: 2-Amino-4-methoxybenzoic acid. 2-Aminoanisic acid. 4-Methoxyanthranilic acid
[4294-95-5]
$C_8H_9NO_3$ 167.164
Plates (EtOH). Mp 166° (dec.) Mp 190°. pK_{a1} 2.06; pK_{a2} 4.88 (25°, 0.1*M* KCl).

N-*(4-Hydroxycinnamoyl) (*E*-): 4-Hydroxy-*N*-(4-hydroxycinnamoyl)anthranilic acid.* ***Avenanthramide G***
$C_{16}H_{13}NO_5$ 299.282
Stress metab. in oats (*Avena sativa*) induced by Victorin M. Cryst. + $^1/_4$ MeOH (MeOH/1% AcOH aq.). Mp

290-291°.

CRC Atlas of Spectral Data and Physical Constants, b843 (*uv*)
Drain, D.G. *et al., J.C.S.*, 1949, 1489 (*synth*)
van der Stelt, C. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1953, **72**, 195 (*synth*)
Jilek, J. *et al., Coll. Czech. Chem. Comm.*, 1985, **50**, 519 (*synth, uv, ir, pmr, deriv*)
Paulidis, V.H. *et al., Synth. Commun.*, 1994, **24**, 533 (*Me ether, synth, ir, pmr, cmr*)
Miyagawa, H. *et al., Phytochemistry*, 1996, **41**, 1473 (*Avenanthramide G*)
Boojamra, C.G. *et al., J.O.C.*, 1997, **62**, 1240-1256 (*Me ether*)

2-Amino-5-hydroxybenzoic acid A-789

5-Hydroxyanthranilic acid
[394-31-0]

$C_7H_7NO_3$ 153.137
Metab. of Tryptophan in rats. Oral hypoglycaemic agent. Violet cryst. (H_2O). Mp 252° dec. pK_{a1} 2.72; pK_{a2} 5.37 (25°, 0.1*M* KCl). Log P 0.66 (calc).

Me ester: [1882-72-0]
$C_8H_9NO_3$ 167.164
Yellow needles. Mp 158°.

Et ester:
$C_9H_{11}NO_3$ 181.191
Cryst. (EtOH). Mp 140°.

8-Methylnonyl ester: Isodecyl 5-hydroxyanthranilate. ***Antibiotic BU 4601A****. BU 4601A*
[148915-76-8]
$C_{17}H_{27}NO_3$ 293.405
Prod. by a *Streptomyces* sp. 5-Lipoxygenase inhibitor. Powder. Sol. MeOH, CCl_4, EtOH, DMSO, EtOAc; fairly sol. hexane; poorly sol. H_2O. λ_{max} 212 (ϵ 29200); 234 (ϵ 9100); 300 (ϵ 3800) (MeOH/HCl) (Derep). λ_{max} 208 (ϵ 33800); 225 (ϵ 24600); 372 (ϵ 4600) (MeOH/NaOH) (Derep). λ_{max} 219 (ϵ 24600); 246 (sh) (ϵ); 360 (ϵ 5200) (MeOH) (Derep).

9-Methyldecyl ester: Isoundecyl 5-hydroxyanthranilate. ***Antibiotic BU 4601B****. BU 4601B*
[148915-77-9]
$C_{18}H_{29}NO_3$ 307.432
Prod. by a *Streptomyces* sp. 5-Lipoxygenase inhibitor. Powder. Sol. MeOH, EtOAc, EtOH, DMSO, CCl_4; fairly sol. hexane; poorly sol. H_2O. λ_{max} 212 (ϵ 29200); 234 (ϵ 9100); 300 (ϵ 3800) (MeOH/HCl) (Derep). λ_{max} 208 (ϵ 33800); 225 (ϵ 24600); 372 (ϵ 4600) (MeOH/NaOH) (Derep). λ_{max} 219 (ϵ 24600); 246 (sh) (ϵ); 360 (ϵ 5200) (MeOH) (Derep).

10-Methylundecyl ester: Isolauryl 5-hydroxyanthranilate. ***Antibiotic BU 4601C****. BU 4601C*
[148915-78-0]
$C_{19}H_{31}NO_3$ 321.459
Prod. by a *Streptomyces* sp. 5-Lipoxygenase inhibitor. Powder. Sol. MeOH, CCl_4, EtOH, DMSO, EtOAc; fairly sol. hexane; poorly sol. H_2O. λ_{max} 212 (ϵ 29200); 234 (ϵ 9100); 300 (ϵ 3800) (MeOH/HCl) (Derep). λ_{max} 208 (ϵ 33800); 225 (ϵ 24600); 372 (ϵ 4600) (MeOH/NaOH) (Derep). λ_{max} 219 (ϵ 24600); 246 (sh) (ϵ); 360 (ϵ 5200) (MeOH) (Derep). λ_{max} 208 (ϵ 33900); 223 (ϵ 4700); 372 (ϵ 4100) (MeOH-NaOH) (Berdy).

N-*(4-Hydroxybenzoyl): 5-Hydroxy-*N-*(4-hydroxybenzoyl)anthranilic acid.* ***Melandrin***
[110846-17-8]
$C_{14}H_{11}NO_5$ 273.245
Constit. of *Melandrium firmum*. Prisms (MeOH). λ_{max} 237 ; 290 ; 336 (MeOH).

N-*(4-Hydroxycinnamoyl)(*E-*): 5-Hydroxy-*N-*(4-hydroxycinnamoyl)anthranilic acid.* ***Avenanthramide A****. Avenalumin I*
[108605-70-5]
$C_{16}H_{13}NO_5$ 299.282
Isol. from the grains of oats (*Avena sativa*). Phytoalexin. Pale yellow needles (Me_2CO aq.). Mp 277°. Darkens at 235°. Originally descr. as Avenalumin I, given the wrong struct. λ_{max} 320 (ϵ 15400); 344 (ϵ 13400) (MeOH/HCl) (Derep). λ_{max} 366 (ϵ 16600) (MeOH/NaOH) (Derep). λ_{max} 317 (ϵ 15200); 336 (ϵ 15900) (MeOH) (Derep).

N-*(4-Hydroxycinnamoyl)(*Z-*):* [116764-20-6]
$C_{16}H_{13}NO_5$ 299.282
Isol. from oats (*Avena sativa*).

N-*(3,4-Dihydroxycinnamoyl)(*E-*):* N-*(3,4-Dihydroxycinnamoyl)-5-hydroxyanthranilic acid.* ***Avenanthramide C***
$C_{16}H_{13}NO_6$ 315.282
Isol. from the grains of *Avena sativa*.

N-*(3,4-Dihydroxycinnamoyl)(*Z-*):*
[116764-22-8]
$C_{16}H_{13}NO_6$ 315.282
Isol. from oats (*Avena sativa*).

N-*(4-Hydroxy-3-methoxycinnamoyl)(*E-*):* N-*Feruloyl-5-hydroxyanthranilic acid.* ***Avenanthramide B****. Avenanthramide 1*
[108605-69-2]
$C_{17}H_{15}NO_6$ 329.309
Isol. from the grains of *Avena sativa*. Long pale yellow needles (Me_2CO aq.). Sol. EtOAc, Et_2O, H_2O-Me_2CO; poorly sol. $CHCl_3$, C_6H_6, H_2O. Mp 246°. λ_{max} 228 ; 315 ; 361 ; 392 (MeOH-NaOH) (Berdy).

N-*(4-Hydroxy-3-methoxycinnamoyl)(*Z-*):* [116764-21-7]
$C_{17}H_{15}NO_6$ 329.309
Isol. from oats (*Avena sativa*).

Me ether: 2-Amino-5-methoxybenzoic acid. 5-Methoxyanthranilic acid
[6705-03-9]
$C_8H_9NO_3$ 167.164
Needles (H_2O). Mp 179-180° (155-156° dec.). pK_{a1} 2.37; pK_{a2} 5.57 (25°, 0.1*M* KCl).

Me ether, nitrile: 2-Amino-5-methoxybenzonitrile, 9CI. 2-Cyano-4-methoxyaniline
[23842-82-2]
$C_8H_8N_2O$ 148.164
Solid. Mp 46°.

Trifluoromethyl ether: 2-Amino-5-(trifluoromethoxy)benzoic acid, 9CI
[83265-56-9]
$C_8H_6F_3NO_3$ 221.136
Needles (H_2O). Mp 137-138°.

Et ether: 2-Amino-5-ethoxybenzoic acid
$C_9H_{11}NO_3$ 181.191
Yellowish solid. Mp 179-180°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1122B (*nmr*)
CRC Atlas of Spectral Data and Physical Constants, 6844 (*uv*)
Puxeddu, E. *et al., Gazz. Chim. Ital.*, 1929, **59**, 14; 492
van der Stelt, C. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1953, **72**, 195
Zeitler, H.J. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1965, **340**, 73 (*synth, props*)
Mitchell, S.C. *et al., J. Chromatogr.*, 1978, **151**, 249
Woo, W.S. *et al., Phytochemistry*, 1987, **26**, 2099 (*Melandrin*)
Collins, F.W. *et al., J. Agric. Food Chem.*, 1989, **37**, 60 (*Avenanthramides*)
Crombie, L. *et al., Tet. Lett.*, 1990, **31**, 2647 (*synth, Avenanthramides*)
Dimberg, L.H. *et al., Cereal Chem.*, 1993, **70**, 637-641 (*Avenanthramides*)
Ohkuma, H. *et al., J. Antibiot.*, 1993, **46**, 705 (*BU 4601*)
Pavlidis, V.H. *et al., Synth. Commun.*, 1994, **24**, 533 (*Me ether*)
Zhang, P. *et al., J. Med. Chem.*, 1995, **38**, 1679 (*Et ether, synth, ir, pmr*)
Ishihara, A. *et al., Phytochemistry*, 1999, **50**, 237-242 (*Avenanthramides, biosynth*)
Leroux, F. *et al., J.O.C.*, 2003, **68**, 4693-4699 (*trifluoromethyl ether, synth, pmr, cmr*)
Manetsch, R. *et al., Chem. Eur. J.*, 2004, **10**, 2487-2506 (*Me ether nitrile*)

3-Amino-5-hydroxybenzoic acid A-790

[76045-71-1]

$C_7H_7NO_3$ 153.137
Key biogenetic precursor of aromatic nuclei in ansamycin, mitomycin and maytansinoid antibiotics.

Hydrochloride: [14206-69-0]
Mp 200-230°.

Me ester: [67973-80-2]
$C_8H_9NO_3$ 167.164
Cryst. (MeOAc/$CHCl_3$). Mp 125-127°.

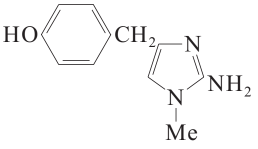
N-*Ac:* [93561-88-7]
$C_9H_9NO_4$ 195.174
Amorph. (MeOH aq.). Mp 245-253°.

Me ether, nitrile: 3-Amino-5-methoxybenzonitrile, 9CI. 3-Cyano-5-methoxyaniline
[269411-71-4]
$C_8H_8N_2O$ 148.164
Yellow solid. Mp 81-85°.

Bickel, H. *et al., Tetrahedron, Suppl.*, No. 8, 1966, 171-179 (*synth*)
Herlt, A.J. *et al., Aust. J. Chem.*, 1981, **34**, 1319 (*synth, ms, pmr*)
Kibby, J.J. *et al., J. Antibiot.*, 1981, **34**, 605 (*isol*)
Becker, A.M. *et al., Tetrahedron*, 1983, **20**, 4189 (*synth, pmr, ms*)
Becker, A.M. *et al., Aust. J. Chem.*, 1984, **37**, 2103-2109 (*use, N-Ac*)
Kim, C.G. *et al., J.A.C.S.*, 1992, **114**, 4941; 1996, **118**, 7486 (*biosynth*)
Watson, T.J.N. *et al., Synth. Commun.*, 1999, **29**, 1379-1382 (*synth, pmr, cmr*)
Reich, S.H. *et al., J. Med. Chem.*, 2000, **43**, 1670-1683 (*Me ether nitrile*)
Clark, J.D. *et al., Org. Process Res. Dev.*, 2004, **8**, 571-575 (*synth*)
Wang, Z. *et al., Bioorg. Med. Chem.*, 2006, **14**, 2242-2252 (*synth, pmr, cmr*)

2-Amino-4-(4-hydroxybenzyl)-1-methyl-1*H*-imidazole A-791

*4-[(2-Amino-1-methyl-1*H*-imidazol-4-yl)methyl]phenol.* ***Dorimidazole A***
[138935-50-9]

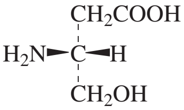


$C_{11}H_{13}N_3O$ 203.243
Alkaloid from the nudibranch *Notodoris gardineri* and *Notodoris citrina*. Anthelminthic, antiparasitic. Yellow powder; cryst. (MeCN) (as hydrobromide). Mp 175-176° (hydrobromide). λ_{max} 228; 269; 297; 300 (MeOH) (Derep). λ_{max} 228; 269; 297; 360 (MeOH) (Berdy).

Alvi, K.A. *et al., J. Nat. Prod.*, 1991, **54**, 1509-1515 (*isol, uv, pmr, cmr, ms, struct, synth*)
Molina, P. *et al., J.O.C.*, 1999, **64**, 2540-2544 (*synth, pmr, cmr*)

3-Amino-4-hydroxybutanoic acid, 9CI A-792

γ-Hydroxy-β-aminobutyric acid. GOBAB
[589-44-6]



$$\begin{array}{c} CH_2COOH \\ H_2N\blacktriangleright C\blacktriangleleft H \\ CH_2OH \end{array}$$

(*R*)-*form*

$C_4H_9NO_3$ 119.12
Antiinflammatory, antifungal and antiseptic agent.

(*R*)-*form* [16504-56-6]

Hydrochloride: [196950-52-4]
Mp 177-178°.

*Lactone: 4-Aminodihydro-2(3*H*)-furanone. β-Amino-γ-butyrolactone*
$C_4H_7NO_2$ 101.105
Mp 175-177° (as hydrochloride). $[\alpha]_D^{20}$ +56.7 (c, 1 in H_2O).

N-*Benzyl, lactone:* [152783-42-1]
$C_{11}H_{13}NO_2$ 191.229
Oil. $[\alpha]_D^{25}$ +16.5 (c, 1.0 in $CHCl_3$).

(*S*)-*form* [16504-57-7] Pharmacol. active isomer.

Lactone: Mp 198-201° (as hydrobromide). $[\alpha]_D^{20}$ -42.6 (c, 1.08 in H_2O).

N-*Benzoyl, lactone:*
$C_{11}H_{11}NO_3$ 205.213
Mp 123.5-126°. $[\alpha]_D^{20}$ -97 (c, 1.41 in $CHCl_3$).

N-tert-*Butyloxycarbonyl, lactone:*
$C_9H_{15}NO_4$ 201.222
Solid. Mp 113-114° (106-108°). $[\alpha]_D^{25}$ -54.3 (c, 1.15 in $CHCl_3$).

N-*Benzyloxycarbonyl, lactone:*
$C_{12}H_{13}NO_4$ 235.239
Cryst. Mp 103-105°. $[\alpha]_D^{20}$ -54.9 (c, 2.27 in $CHCl_3$).

N-*Trifluoroacetyl, benzyl ester:* [673470-50-3]
$C_{13}H_{14}F_3NO_4$ 305.253
Cryst. solid. Mp 70-71°. $[\alpha]_D^{22.5}$ +9.1 (c, 0.99 in $CHCl_3$).

(±)-*form* [16504-55-5]
Needles. Mp 184°.

Lactone: [16504-58-8]
Mp 185-186° (as hydrochloride).

Lactone, N-*benzyl:* [157037-11-1]
$C_{11}H_{13}NO_2$ 191.229
Oil.

(ξ)-*form*

O-*(4-Hydroxybenzoyl),* N,N,N-*tri-Me, betaine: 1-Carboxy-3-[(4-hydroxybenzoyl)oxy]-*N,N,N-*trimethyl-2-propanaminium inner salt, 9CI.* ***Zooxanthellabetaine A***
[208256-89-7]
$C_{14}H_{19}NO_5$ 281.308
Isol. from the cultures of a symbiotic dinoflagellate *Symbiodinium* sp. Oil. $[\alpha]_D^{20}$ -13 (c, 0.0035 in MeOH).

Jolles, P. *et al., Bull. Soc. Chim. Fr.*, 1951, 862-863 (*synth*)
Chibnall, A.C. *et al., Biochem. J.*, 1958, **68**, 122-128 (*synth*)
Nagai, K. *et al., Arzneim.-Forsch.*, 1967, **17**, 1575-1577 (*synth, isomers, pharmacol*)
Kim, Y.B. *et al., Arch. Pharmacal Res.*, 1985, **8**, 1-6; *CA*, **103**, 98858d (*cryst struct*)
McGarvey, G.J. *et al., J.A.C.S.*, 1986, **108**, 4943-4952 (*lactone N-benzyloxycarbonyl, synth, ir, pmr*)
Hvidt, T. *et al., Can. J. Chem.*, 1988, **66**, 779-782 (*synth, pmr, cmr*)
Hanessian, S. *et al., Can. J. Chem.*, 1993, **71**, 1407-1411 (*lactone, N-tert-butyloxycarbonyl, synth, ir, pmr*)
Maude, A.B. *et al., J.C.S. Perkin 1*, 1997, 2513-2526 (*synth, ir, pmr*)
Calvisi, G. *et al., Synlett*, 1997, 71-74 (*lactone, synth, pmr*)
Nakamura, H. *et al., Bull. Chem. Soc. Jpn.*, 1998, **71**, 781-787 (*Zooanthellabetaine A*)
El Hadri, A. *et al., J. Med. Chem.*, 2002, **45**, 2824-2831 (*N-benzyl lactone, synth*)
Jackson, R.F.W. *et al., Org. Biomol. Chem.*, 2004, **2**, 110-113 (*N-trifluoroacetyl benzyl ester, synth, pmr, cmr*)

1-Amino-3-hydroxy-8-decen-5-one A-793

$H_3CCH{=}CHCH_2CH_2COCH_2$-
$CH(OH)CH_2CH_2NH_2$
$C_{10}H_{19}NO_2$ 185.266

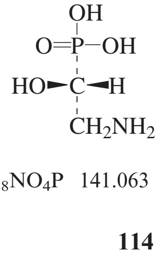
(+)-(*E*)-*form*

N-*Ac:* ***Streptenol E***
$C_{12}H_{21}NO_3$ 227.303
Prod. by *Streptomyces* sp. strain A1. Oil. $[\alpha]_D^{22}$ +33 (c, 0.34 in $CHCl_3$).

Puder, C. *et al., J. Nat. Prod.*, 2001, **64**, 42-45

(2-Amino-1-hydroxyethyl)phosphonic acid, 9CI A-794

[41744-58-5]



$$\begin{array}{c} OH \\ O{=}P{-}OH \\ HO\blacktriangleright C\blacktriangleleft H \\ CH_2NH_2 \end{array}$$

(*R*)-*form*

$C_2H_8NO_4P$ 141.063

(*R*)-*form* [115511-00-7]
Isol. from the plasma membrane of *Acanthamoeba castellanii*. Cryst. (EtOH aq.). Mp 244-246° dec. $[\alpha]_D^{20}$ -31.4 (c, 0.52 in H_2O).

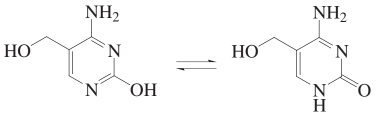
(*S*)-*form* [121421-25-8]
Cryst. (EtOH aq.). Mp 245-247° dec. $[\alpha]_D^{22}$ +32.5 (c, 1 in H_2O).

(±)-*form* [114157-09-4]
Cryst. (EtOH aq.). Mp 260-262° dec.

Korn, E.D. *et al., J. Biol. Chem.*, 1973, **248**, 2257 (*isol*)
Hammerschmidt, F. *et al., Annalen*, 1988, 537-542; 955-960; 961-964; 1989, 577-583 (*synth, abs config*)
Heisler, A. *et al., Tetrahedron: Asymmetry*, 1993, **4**, 959-960 (*synth*)

4-Amino-2-hydroxy-5-(hydroxymethyl)pyrimidine A-795

*4-Amino-2-hydroxy-5-pyrimidinemethanol. 4-Amino-5-hydroxymethyl-2(1*H*)-pyrimidinone. 5-Hydroxymethylcytosine*
[1123-95-1]



$C_5H_7N_3O_2$ 141.129
DNA constit. of various plants and viruses. Cryst. + $0.5H_2O$ (H_2O). Mp 300° dec. pK_{a1} 4.32; pK_{a2} 13.

OH-form

2-Me ether: 4-Amino-5-(hydroxymethyl)-2-methoxypyrimidine. 4-Amino-2-methoxy-5-pyrimidinemethanol. ***Bacimethrin***
$C_6H_9N_3O_2$ 155.156
Prod. by *Bacillus megaterium* and *Streptomyces albus*. Active against gram-positive and -negative bacteria. Thiamine antagonist. Needles (MeOH or EtOH/Et_2O). Sol. H_2O, MeOH, AcOH; fairly sol. EtOH, Py; poorly sol. butanol, hexane. Mp 175°. λ_{max} 230 (ϵ 8540); 263 (ϵ 9590) (0.1*M* HCl) (Derep). λ_{max} 228 (ϵ 8760); 271 (ϵ 8170) (0.1*M* NaOH) (Derep). λ_{max} 228 (ϵ 8310); 270 (ϵ 7630) (H_2O) (Derep). λ_{max} 229 (ϵ 6600); 273 (ϵ 6200) (MeOH) (Berdy).

▶ LD_{50} (mus, ivn) 300 mg/kg.

2-Me ether, O-*Ac:*
$C_8H_{11}N_3O_3$ 197.193
Mp 131°.

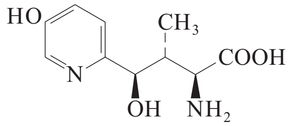
2-Me ether, O,N-*Di-Ac:*
$C_{10}H_{13}N_3O_4$ 239.23
Mp 142°.

Wyatt, G.R. *et al., Biochem. J.*, 1953, **55**, 774 (*isol*)
Miller, C.S. *et al., J.A.C.S.*, 1955, **77**, 752 (*synth, uv*)
Tanaka, F. *et al., J. Antibiot., Ser. A*, 1961, **14**, 161 (*Me ether, isol, struct*)
Koppel, H.C. *et al., J.O.C.*, 1962, **27**, 1492; 3614 (*Me ether, synth, uv*)
Drautz, M. *et al., J. Antibiot.*, 1987, **40**, 1431 (*Me ether, isol, synth, props*)
Isono, K. *et al., J. Antibiot.*, 1988, **41**, 1711 (*rev*)

Hudson, R.H.E. *et al., Can. J. Chem.*, 2007, 302-312 (*synth, pmr, cmr*)

2-Amino-4-hydroxy-4-(5-hydroxy-2-pyridinyl)-3-methylbutanoic acid A-796

α-Amino-γ,5-dihydroxy-β-methyl-2-pyridinebutanoic acid, 9CI



$C_{10}H_{14}N_2O_4$ 226.232

(2*S*,3*R*,4*R*)-*form* [76249-78-0]
Amino acid residue from Nikkomycin Z, N-218.

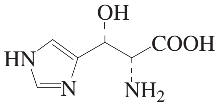
(2*S*,3*S*,4*S*)-*form*
Nikkomycin D
[67676-66-8]
The terminal amino acid of the nikkomycins and neopolyoxins. Fine needles (H_2O). Mp 230° dec Mp 207° dec. $[\alpha]^{20}_{D}$ -13.4 (c, 0.59 in H_2O).

[76612-52-7 , 83572-53-6 , 83572-54-7 , 83572-56-9 , 83572-55-8]

Koenig, W.A. *et al., Annalen*, 1980, 1728; 1982, 1615 (*isol, synth, cryst struct*)
Teintze, M. *et al., Biochemistry*, 1981, **20**, 6446 (*isol*)
Uramoto, M. *et al., Tetrahedron*, 1982, **38**, 1599 (*isol*)

2-Amino-3-hydroxy-3-(4-imidazolyl)propanoic acid A-797

β-Hydroxyhistidine, 9CI



(2*R*,3*R*)-*form*

$C_6H_9N_3O_3$ 171.155

(2*R*,3*R*)-*form*
D-threo-*form*
[35849-15-1 (hydrochloride)]
Pale yellow cryst. (as hydrochloride). $[\alpha]^{25}_{D}$ +15 (c, 1.2 in H_2O) (hydrochloride).

N^{α}-*Ac:* $[\alpha]^{25}_{D}$ -17 (c, 1.25 in H_2O).

(2*S*,3*R*)-*form*
L-erythro-*form*
[41215-80-9]
[51077-31-7 (hydrochloride)]
Component of antibiotics of the Bleomycin A_2 group. Cryst. Mp 205° dec. $[\alpha]^{28}_{D}$ +40 (c, 1 in H_2O) (hydrochloride).

(2*S*,3*S*)-*form*
L-threo-*form*
[148219-09-4]
Constit. of a pyoverdin isol. from *Pseudomonas fluorescens* 244. Pale yellow solid. $[\alpha]_D$ -9 (c, 1 in H_2O).

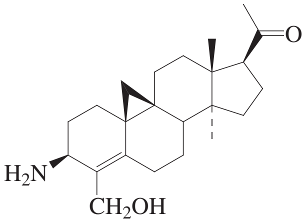
(2*RS*,3*RS*)-*form*
(±)-threo-*form*
[35849-17-3]
Solid (as hydrochloride). CAS no. refers to hydrochloride.

(2*RS*,3*SR*)-*form*
(±)-erythro-*form*
[71389-30-5]
Cryst. Mp 205° dec.

Hydrochloride: [35849-19-5]
Needles (2-propanol/EtOH aq.). Mp 228°.

Takita, T. *et al., J. Antibiot.*, 1971, **24**, 795 (*isol, nmr, struct, synth*)
Ohashi, Y. *et al., Agric. Biol. Chem.*, 1973, **37**, 2283 (*isol*)
Koyama, G. *et al., J. Antibiot.*, 1973, **26**, 109 (*cryst struct*)
Naganawa, H. *et al., J. Antibiot.*, 1977, **30**, 388 (*cmr*)
Hecht, S.M. *et al., J.A.C.S.*, 1979, **101**, 3982 (*synth, pmr*)
Owa, T. *et al., Chem. Lett.*, 1988, 83; 1873 (*synth*)
Hancock, D.K. *et al., Chem. Comm.*, 1993, 468 (*isol, pmr, cmr*)
Dong, L. *et al., J.O.C.*, 2002, **67**, 4759-4770 (*S,S-form, synth, pmr, cmr*)

3-Amino-4-hydroxymethyl-14-methyl-9,19-cyclopregn-4-en-20-one A-798

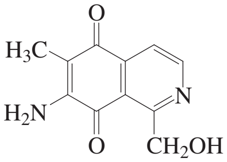


$C_{23}H_{35}NO_2$ 357.535

3β-*form*
N-*Me:* ***30-Hydroxycyclomicrobuxene***
[220705-48-6]
$C_{24}H_{37}NO_2$ 371.562
Alkaloid from the roots of *Buxus sempervirens*. Amorph. solid. $[\alpha]^{20}_{D}$ +84 (c, 0.69 in $CHCl_3$). Misleading synonym. λ_{max} 202 (MeOH).

Atta-ur-Rahman, *et al., Nat. Prod. Lett.*, 1998, **12**, 299-306 (*isol, pmr, cmr*)

7-Amino-1-hydroxymethyl-6-methyl-5,8-isoquinolinedione, 9CI A-799



$C_{11}H_{10}N_2O_3$ 218.212

O-*Angeloyl:* ***Cribrostatin 3***
[276682-84-9]
$C_{16}H_{16}N_2O_4$ 300.313
Alkaloid from *Cribrochalina* sp. Cytotoxic agent. Orange-red needles (CH_2Cl_2/MeOH). Mp 190-192°.

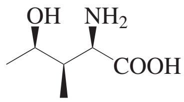
N^7-*Me,* O-*angeloyl:* ***Cribrostatin 5***
[276682-90-7]
$C_{17}H_{18}N_2O_4$ 314.34
Alkaloid from *Cribrochalina* sp. Cytotoxic agent. Red-brown plates (MeOH/CH_2Cl_2).

N^7-*(2-Sulfoethyl),* O-*angeloyl:* ***Cribrostatin 7***
[683276-94-0]
$C_{18}H_{20}N_2O_7S$ 408.431
Alkaloid from a *Petrosia* sp. Cytotoxic agent. Dark red film. λ_{max} 210 (ε 14500); 282 (ε 6500); 338 (ε 2000); 474 (ε 1700) (MeOH).

Pettit, G.R. *et al., J. Nat. Prod.*, 2000, **63**, 793-798 (*Cribrostatin 3, Cribrostatin 5*)
Sandoval, I.T. *et al., Nat. Prod. Res.*, 2004, **18**, 89-93 (*Cribrostatin 7*)

2-Amino-4-hydroxy-3-methylpentanoic acid A-800

2-Amino-2,3,5-trideoxy-3-methylpentonic acid. 4-Hydroxyisoleucine
[50764-07-3]



(2*R*,3*R*,4*R*)-*form*

$C_6H_{13}NO_3$ 147.174

(2*R*,3*R*,4*R*)-*form*
D-xylo-*form. 2-Amino-2,3,5-trideoxy-3-methyl-D-xylonic acid*
[60010-78-8]
Cryst. (EtOH aq.). Mp *ca.*° 230. $[\alpha]^{20}_{D}$ -35.6 (c, 1.2 in D_2O).

*1,4-Lactone: 3-Aminodihydro-4,5-dimethyl-2(3*H*)-furanone*
$C_6H_{11}NO_2$ 129.158
Cryst. (EtOH/petrol) (as hydrochloride). Mp 222° (hydrochloride). $[\alpha]^{25}_{D}$ +88.7 (c, 1 in MeOH).

1,4-Lactone, N-*Ac:*
Needles (EtOH). Mp 140°. $[\alpha]^{25}_{D}$ +88 (c, 1 in DMSO).

(2*R*,3*R*,4*S*)-*form*
L-arabino-*form. 2-Amino-2,3,5-trideoxy-3-methyl-L-arabinonic acid*
[60010-73-3]
Minor amino acid constit. of *Trigonella foenum-graecum* (fenugreek) seeds. $[\alpha]^{20}_{D}$ +1 (c, 1 in H_2O). Orginally thought to be the 2*R*,3*R*,4*R*-form.

1,4-Lactone:
Cryst. (as hydrochloride). Mp 170-175° (hydrochloride).

1,4-Lactone, N-*Ac: 3-Acetamidodihydro-4,5-dimethyl-2(3*H*)-furanone.* ***Desmodilactone***
[60010-74-4]
$C_8H_{13}NO_3$ 171.196
Constit. of *Desmodium styracifolium*. Component of Guang Jin Qian Cao. Cryst. Mp 84-85°. $[\alpha]^{18}_{D}$ -16.4 (c, 0.11 in MeOH).

(2*S*,3*R*,4*R*)-*form*
D-lyxo-*form. 2-Amino-2,3,5-trideoxy-3-methyl-D-lyxonic acid*
[55399-92-3]
Cryst. (EtOH aq.). Mp *ca.*° 220. $[\alpha]^{20}_{D}$ -

24.9 (c, 1.17 in D_2O).

1,4-Lactone:
Needles (EtOH/petrol) (as hydrochloride). Mp 255° (hydrochloride). $[\alpha]_D^{25}$ +24.3 (c, 1 in MeOH).

1,4-Lactone, N-*Ac:*
Needles (EtOH). Mp 141°.

(2S,3R,4S)-form
L-ribo-*form. 2-Amino-2,3,5-trideoxy-3-methyl-*L*-ribonic acid*
[55399-93-4]
Major constit. of *Trigonella foenum-graecum* (fenugreek). Cryst. (EtOH aq.). Mp 224-225°. $[\alpha]_D^{20}$ +31 (c, 1 in H_2O). Stereochem. revised in 1989.

1,4-Lactone:
Needles (EtOH/petrol) (as hydrochloride). Mp 230° (hydrochloride). $[\alpha]_D^{25}$ -15.5 (c, 1 in MeOH).

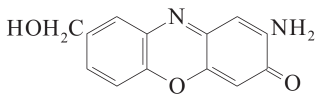
1,4-Lactone, N-*Ac:*
Needles (EtOH). Mp 94°.

(2S,3S,4R)-form
D-arabino-*form. 2-Amino-2,3,5-trideoxy-3-methyl-*D*-arabinonic acid*
[21704-86-9]
Constit. of the flowers of *Quararibea funebris*. Mp 205-207°. $[\alpha]_D^{27}$ +2.9 (c, 0.1 in H_2O). λ_{max} 197 (ϵ 250) (H_2O).

1,4-Lactone: [71392-28-4]
[90693-46-2]
Constit. of the flowers of *Quararibea funebris*. Powder (as hydrochloride). Mp 212-215° (hydrochloride). $[\alpha]_D^{25}$ -14.8 (c, 0.7 in MeOH).

Fowden, L. *et al., Phytochemistry*, 1973, **12**, 1707-1711 (*Trigonella foenum-graecum constits*)
Gieren, A. *et al., Annalen*, 1974, 1561-1569 (*synth*)
Hasan, M. *et al., Annalen*, 1976, 781-787 (*lactone, synth, pmr*)
Raffauf, R.F. *et al., J.O.C.*, 1984, **49**, 2714-2718 (*Quararbea funebris constit*)
Alcock, N.W. *et al., Phytochemistry*, 1989, **28**, 1835-1841 (*struct*)
Inghardt, T. *et al., Tetrahedron*, 1991, **47**, 6469-6482 (*synth, abs config, cryst struct*)
Yang, J. *et al., Yaoxue Xuebao*, 1993, **28**, 197-201; *CA*, **119**, 156209m (*Desmodilactone*)
Wang, Q. *et al., Eur. J. Org. Chem.*, 2002, 834-839 (*synth, pmr, cmr*)
Rolland-Fulcrand, V. *et al., Eur. J. Org. Chem.*, 2004, 873-877 (*synth, pmr, cmr*)
Aouadi, K. *et al., Synthesis*, 2007, 3399-3405 (*2S,3R,4R-form, synth, pmr, cmr, ms*)

2-Amino-8-(hydroxymethyl)-3*H*-phenoxazin-3-one A-801



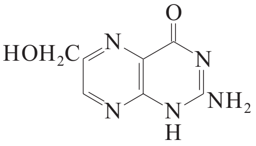
$C_{13}H_{10}N_2O_3$ 242.234

N-*Ac: 2-Acetamido-8-(hydroxymethyl)-3*H*-phenoxazin-3-one.* ***Exfoliazone****. BT 38. Antibiotic BT 38*
[132627-73-7]
$C_{15}H_{12}N_2O_4$ 284.271
Prod. by *Streptomyces exfoliatus*. Active against *Valsa ceratosperma*. Orange needles ($CHCl_3$). Sol. MeOH, $CHCl_3$, EtOAc; poorly sol. H_2O, butanol. Mp 294-296°. λ_{max} 238 (ϵ 75300); 400 (ϵ 42300) (solvent not reported) (Derep). λ_{max} 238 (ϵ 75300); 400 (ϵ 42300) (MeOH) (Berdy).

Imai, S. *et al., J. Antibiot.*, 1990, **43**, 1606

2-Amino-6-(hydroxymethyl)-4(1*H*)-pteridinone, 9CI A-802

6-Hydroxymethylpterin. ***Ranachrome 3****. 2-Amino-4-hydroxy-6-(hydroxymethyl)pteridine*
[712-29-8]



$C_7H_7N_5O_2$ 193.165
Occurs widely in nature. The 7,8-dihydro deriv. is the biological precursor of folic acid. Cryst. (H_2O). Mp 320° dec.

▶ UO3450000

O-*[4-*O*-Methyl-α-*D*-glucuronopyranosyl-(1→6)-β-*D*-galactopyranoside]:* ***Cyanopterin***
[223532-84-1]
$C_{20}H_{27}N_5O_{13}$ 545.459
Isol. from *Synechocystis* sp. PCC 6803. λ_{max} 192 ; 236 ; 276 ; 345 (H_2O).

O-*Ac:* [73978-45-7]
$C_9H_9N_5O_3$ 235.202
Cryst. (H_2O). Mp 300° dec.

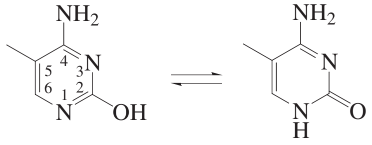
N^2,O-*Di-Ac:* [32363-58-9]
$C_{11}H_{11}N_5O_4$ 277.239
Cryst. (Me_2CO). Mp 239-242° dec. (227-229°).

[1501-52-6]

Blair, J.A. *et al., Org. Mass Spectrom.*, 1969, **2**, 923 (*ms*)
Thijssen, H.H.W. *et al., Anal. Biochem.*, 1973, **54**, 609 (*synth*)
Boyle, P.H. *et al., Chem. Ber.*, 1980, **113**, 1514 (*synth, uv, pmr*)
Waring, P. *et al., Aust. J. Chem.*, 1985, **38**, 629 (*synth, bibl*)
Zeitler, H.J. *et al., Methods Enzymol.*, 1986, **122**, 273 (*rev, hplc*)
Burgmayer, S.J.N. *et al., Inorg. Chem.*, 1988, **27**, 4059 (*ir*)
Lee, H.W. *et al., Biochim. Biophys. Acta*, 1999, **1410**, 61-70 (*Cyanopterin*)

4-Amino-2-hydroxy-5-methylpyrimidine A-803

*4-Amino-5-methyl-2(1*H*)-pyrimidinone, 9CI. 4-Amino-5-methyl-2-pyrimidinol. 5-Methylcytosine*
[554-01-8]



$C_5H_7N_3O$ 125.13
Constit. of DNA of plants and animals. Cryst. (H_2O). Mp 287-292°.

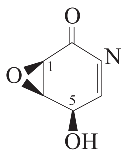
Hydrochloride:
Plates or prisms. Mp 288-290°.

*1-β-*D*-(2,3-Dideoxyribofuranosyl): 2′,3′-Dideoxy-5-methylcytidine, 9CI*
[107036-56-6]
$C_{10}H_{15}N_3O_3$ 225.247
Lyophilised solid.

Fox, J.J. *et al., J.A.C.S.*, 1951, **73**, 3256 (*synth*)
Kream, J. *et al., J.A.C.S.*, 1952, **74**, 5157 (*isol*)
Thomas, A.J. *et al., Biochem. J.*, 1956, **62**, 1 (*isol*)
Kokko, J. *et al., J.A.C.S.*, 1962, **84**, 1042 (*pmr*)
Rice, J.M. *et al., J.A.C.S.*, 1965, **87**, 4569 (*ms*)
Kloetzer, W. *et al., Monatsh. Chem.*, 1965, **96**, 1721 (*synth*)
Padmaja, N. *et al., Acta Cryst. C*, 1987, **43**, 2157 (*cryst struct*)
Kim, C.H. *et al., J. Med. Chem.*, 1987, **30**, 862 (*β-*D*-2,3-dideoxyribofuranosyl, synth, pmr, ms*)
Buchini, S. *et al., Eur. J. Org. Chem.*, 2006, 3152-3168 (*synth, pmr, cmr, ms*)

3-Amino-5-hydroxy-7-oxabicyclo[4.1.0]hept-3-en-2-one, 9CI A-804

2-Amino-5,6-epoxy-4-hydroxy-2-cyclohexen-1-one



(1*R*,5*R*,6*R*)−*form*

$C_6H_7NO_3$ 141.126

(1R,5R,6R)-form
N-*Ac: Antibiotic MT 35214. MT 35214*
[89020-32-6]
$C_8H_9NO_4$ 183.163
Semisynthetic. Weakly active against gram-positive and -negative bacteria and *Candida* spp. Prisms (Me_2CO/Et_2O). Mp 149-151° dec. $[\alpha]_D^{20}$ +104 (c, 1 in MeOH). λ_{max} 265 (ϵ 5910); 321 (ϵ 12700) (0.1*N* NaOH) (Derep). λ_{max} 212 (ϵ 11000); 276 (ϵ 3510) (H_2O) (Derep).

N-*Ac, 5-ketone: 3-(Acetylamino)-7-oxabicyclo[4.1.0]hept-3-ene-2,5-dione. 2-(Acetylamino)-5,6-epoxy-2-cyclohexene-1,4-dione. Antibiotic MT 36531. MT 36531*
[89020-31-5]
$C_8H_7NO_4$ 181.148
Semisynthetic. Shows weak antibacterial activity. Needles (EtOAc/Et_2O). Mp 144-145°. $[\alpha]_D^{20}$ -99 (c, 0.5 in MeOH).

(1S,5S,6S)-form
Antibiotic MM 14201*. MM 14201*
[89020-30-4]
Isol. from *Streptomyces* spp. Sol. MeOH, H_2O; poorly sol. hexane. $[\alpha]_D^{20}$ -202 (c, 0.334 in MeOH). λ_{max} 304 (H_2O) (Derep). λ_{max} 304 (EtOH) (Berdy).

N-*Ac:* N-*(5-Hydroxy-2-oxo-7-oxabicyclo[4.1.0]hept-3-en-3-yl)acetamide.* ***Antibiotic LL C10037α****. LL C10037α*

[93752-54-6]
$C_8H_9NO_4$ 183.163
Isol. from *Streptomyces* spp. Shows antitumour props. Weakly active against bacteria. Fluffy powder. Sol. H_2O, MeOH, EtOH; poorly sol. Me_2CO, hexane. Mp 153°. $[\alpha]_D^{26}$ -155 (c, 0.1 in H_2O). $[\alpha]_D^{20}$ -202 (c, 0.3 in MeOH). Revised struct. λ_{max} 265 (ϵ 5910); 321 (ϵ 12700) (0.1*N* NaOH) (Derep). λ_{max} 212 (ϵ 11000); 276 (ϵ 3510) (H_2O) (Derep). λ_{max} 212 (ϵ 10970); 275 (ϵ 3510) (H_2O) (Berdy). λ_{max} 265 (ϵ 5200); 321 (ϵ 15200) (NaOH) (Berdy).

(1RS,5RS,6RS)-form

N-*Ac:* [157183-80-7]
Cryst. (Me_2CO/Et_2O). Mp 167° dec.

N-*Ac, 5-ketone:*
Pale yellow solid (EtOAc/petrol). Mp 169-170° dec.

(1RS,5SR,6RS)-form

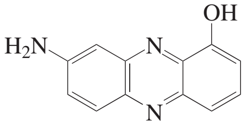
N-*Ac: (±)-Epi-LL-C10037α*
[157183-81-8]
Mp 154° dec.

[121055-94-5 , 121055-92-3]

Box, S.J. *et al., J. Antibiot.*, 1983, **36**, 1631 (*isol, props*)
Lee, M.D. *et al., J. Antibiot.*, 1984, **37**, 1149 (*isol, struct*)
Whittle, Y.G. *et al., J.A.C.S.*, 1987, **109**, 5043 (*biosynth, struct*)
Gould, S.J. *et al., J.A.C.S.*, 1989, **111**, 7932 (*biosynth*)
Shen, B. *et al., J.O.C.*, 1990, **55**, 4422 (*pmr, cryst struct*)
Wipf, P. *et al., J.O.C.*, 1994, **59**, 3520 (*synth, LL C10037*)
Wipf, P. *et al., Synthesis*, 1995, 1549 (*synth*)
Kapfer, I. *et al., Tet. Lett.*, 1996, **37**, 2101 (*synth, LL C10037α*)
Taylor, R.J.K. *et al., Synthesis*, 1998, 775-790 (*synth, LL-C10037α, 5-ketone, ir, pmr, cmr, ms*)
Macdonald, G. *et al., Tet. Lett.*, 1998, **39**, 5433-5436 (*synth*)
Murphy, S.T. *et al., Org. Lett.*, 1999, **1**, 1483-1485 (*synth, LL C10037α*)
Block, O. *et al., J.O.C.*, 2000, **65**, 716-721 (*synth, LL C10037α*)

8-Amino-1-hydroxyphenazine A-805

8-Amino-1-phenazinol, 9CI

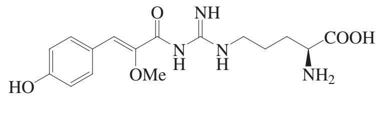


$C_{12}H_9N_3O$ 211.223
Prod. by an unidentified bacterium. λ_{max} 275 ; 376 ; 480 (MeOH) (Berdy).

Me ether: 8-Amino-1-methoxyphenazine
[23448-77-3]
$C_{13}H_{11}N_3O$ 225.249
Bright orange solid. Mp 180° Mp 240-243° (dec.) (double Mp). λ_{max} 275 ; 376 ; 480 (EtOH).

Gerber, N.N. *et al., J. Het. Chem.*, 1969, **6**, 297-300 (*isol*)

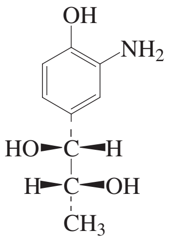
2-Amino-5-[[[[3-(4-hydroxyphenyl)-2-methoxy-2-propenoyl]amino](imino)methyl]amino]pentanoic acid A-806



$C_{16}H_{22}N_4O_5$ 350.374
Isol. from the ascidian *Atriolum robustum*. Amorph. solid. $[\alpha]_D^{25}$ -3.2 (c, 0.15 in H_2O). λ_{max} 295 (ϵ 34000) (H_2O).

Kehraus, S. *et al., J. Med. Chem.*, 2004, **47**, 2243-2255 (*isol*)

1-(3-Amino-4-hydroxyphenyl)-1,2-propanediol A-807



$C_9H_{13}NO_3$ 183.207

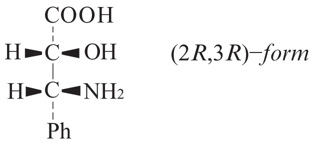
(1R,2R)-form

4′-Me ether, N-*Ac:* ***Agaridiol***
[243864-56-4]
$C_{12}H_{17}NO_4$ 239.271
Prod. by an *Agaricus* sp. Antibacterial agent.

Berg, A. *et al., J. Basic Microbiol.*, 1999, **39**, 213-215

3-Amino-2-hydroxy-3-phenylpropanoic acid A-808

β-Amino-α-hydroxybenzenepropanoic acid, 9CI. 3-Amino-3-phenyllactic acid. 3-Phenylisoserine
[6049-55-4]



$C_9H_{11}NO_3$ 181.191

(2R,3S)-form

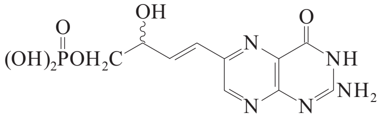
(-)-threo-*form*
[136561-53-0] Residue present in, and intermed. in synth. of, the sidechain of Taxol, T-52.
Solid. Mp 224-226° Mp 238° dec. (as hydrochloride). $[\alpha]_D$ -14.9 (c, 0.55 in 6*M* HCl). $[\alpha]_D^{25}$ -14.5 (c, 0.37 in MeOH) (as hydrochloride).

N-*Benzoyl:* [132201-33-3]
$C_{16}H_{15}NO_4$ 285.299
Isol. from *Taxus baccata*. Sidechain of Taxol, T-52. Cryst. (EtOAc). Mp 177-178° (166-168°). $[\alpha]_D^{25}$ -36.3 (c, 0.73 in EtOH). $[\alpha]_D^{25}$ -31.7 (c, 1.0 in EtOH).

Harada, K. *et al., J.O.C.*, 1966, **31**, 1407 (*abs config*)
Kamandi, E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1974, **307**, 871-878 (*synth, amide*)
Harada, K. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 2911 (*synth, abs config*)
Bruncko, M. *et al., Angew. Chem., Int. Ed.*, 1997, **36**, 1483-1486 (*synth, 2R,3S-form*)
Zhou, Z. *et al., Synth. Commun.*, 2001, **31**, 3609-3615; 2003, **33**, 723-728 (*synth, ir, pmr, amide, N-benzoyl*)

2-Amino-6-[3-hydroxy-4-(phosphonooxy)-1-butenyl]-4(1*H*)-pteridinone, 9CI A-809

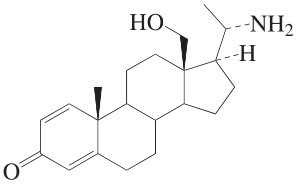
2-Amino-4-hydroxy-6-(3-hydroxy-4-phosphonooxy-1-butenyl)pteridine
[136338-57-3]



$C_{10}H_{12}N_5O_6P$ 329.208
Isol. from *Rhodopseudomonas sphaeroides.*

Seo, N. *et al., Biochim. Biophys. Acta*, 1991, **1074**, 439 (*isol, synth*)

20-Amino-18-hydroxypregna-1,4-dien-3-one A-810



$C_{21}H_{31}NO_2$ 329.481

(20S)-form

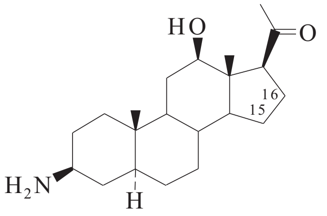
N-*Me:* ***18-Hydroxy-20-(methylamino)-pregna-1,4-dien-3-one***
[113846-36-9]
$C_{22}H_{33}NO_2$ 343.508
Alkaloid from the leaves of *Didymeles madagascariensis* (Didymelaceae). $[\alpha]_D$ +31 (c, 1.71 in EtOH).

N,N-*Di-Me:* ***20-(Dimethylamino)-18-hydroxypregna-1,4-dien-3-one***
[91147-28-3]
$C_{23}H_{35}NO_2$ 357.535
Alkaloid from the stem bark of *Didymeles madagascariensis* (Didymelaceae). λ_{max} 241 (log ϵ 4.39); 322 (log ϵ 4.07) (EtOH).

18-Aldehyde, N,N-*di-Me:* ***20-(Dimethylamino)-3-oxopregna-1,4-dien-18-al***
[91147-29-4]
$C_{23}H_{33}NO_2$ 355.519
Alkaloid from the stem bark of *Didymeles madagascariensis* (Didymelaceae). Cryst. (Et_2O). Mp 157°. $[\alpha]_D$ +69 (c, 0.01 in $CHCl_3$).

Sánchez, V. *et al., Bull. Soc. Chim. Fr.*, Part II, 1984, 71; 1987, 877 (*isol, uv, cd, pmr, cmr, ms, struct*)

3-Amino-12-hydroxypregnan-20-one A-811



$C_{21}H_{35}NO_2$ 333.513

(3β,5α,12β)-*form*
Bokitamine
[5224-04-4]
Alkaloid from a *Holarrhena* sp. (poss. *Holarrhena wulfsbergii*) (Apocynaceae). Cryst. (EtOAc). Mp 191°.

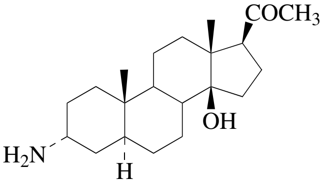
N-*Ac:*
$C_{23}H_{37}NO_3$ 375.55
Mp 247-248°. $[\alpha]_D$ +22.5 ($CHCl_3$).

N,O-*Di-Ac:*
$C_{25}H_{39}NO_4$ 417.587
Mp 202-204°.

15,16-Didehydro: 3-Amino-12-hydroxypregn-15-en-20-one. ***Kisantamine***
[69375-36-6]
$C_{21}H_{33}NO_2$ 331.497
Alkaloid from *Holarrhena congolensis* (Apocynaceae). $[\alpha]_D^{20}$ -16 (c, 0.1 in $CHCl_3$) (as *N*-Ac).

Nellé, S. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1970, **271**, 153 (*isol, struct, synth*)
Dadoun, H. *et al., Plant. Med. Phytother.*, 1978, **12**, 225; *CA*, **90**, 100106r (*deriv*)

3-Amino-14-hydroxypregnan-20-one A-812

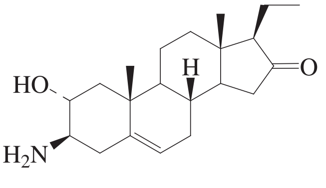


$C_{21}H_{35}NO_2$ 333.513

(3α,5α,14β)-*form* [215595-77-0]
Alkaloid from *Holarrhena curtisii*. Cytotoxic and leishmanicidal agent. Amorph. $[\alpha]_D$ +23.3 (c, 0.26 in $CHCl_3$).

Kam, T.-S. *et al., J. Nat. Prod.*, 1998, **61**, 1332-1336 (*isol, pmr, cmr, ms*)

3-Amino-2-hydroxypregn-5-en-16-one A-813



$C_{21}H_{33}NO_2$ 331.497

(2α,3β)-*form*

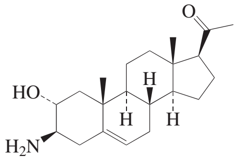
N-*Me: 2-Hydroxy-3-(methylamino)-pregn-5-en-16-one.* ***Kurchiphyllamine***
[1433-87-0]
$C_{22}H_{35}NO_2$ 345.524
Alkaloid from the leaves of *Holarrhena antidysenterica* (Apocynaceae). Mp 161°. $[\alpha]_D$ -211 (c, 1.3 in $CHCl_3$).

N,N-*Di-Me: 3-(Dimethylamino)-2-hydroxypregn-5-en-16-one.* ***Kurchiphylline***
[1433-88-1]
$C_{23}H_{37}NO_2$ 359.551
Alkaloid from the leaves of *Holarrhena antidysenterica* (Apocynaceae). Mp 184°. $[\alpha]_D$ -173 (c, 1 in $CHCl_3$).

N,N-*Di-Me,* O-*Ac:* Mp 125°.

Janot, M.-M. *et al., Bull. Soc. Chim. Fr.*, 1966, 1212-1216 (*Kuchiphyllamine, Kurchiphylline*)

3-Amino-2-hydroxypregn-5-en-20-one A-814



Absolute Configuration

$C_{21}H_{33}NO_2$ 331.497

(2α,3β)-*form*

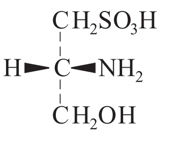
N,N-*Di-Me: 3-(Dimethylamino)-2-hydroxypregn-5-en-20-one.* ***Kurchiline***
$C_{23}H_{37}NO_2$ 359.551
Alkaloid from the leaves of *Holarrhena antidysenterica* (Apocynaceae). Mp 219°. $[\alpha]_D$ +46 (c, 1 in $CHCl_3$).

N,N-*Di-Me,* O-*Ac:* Mp 139°.

Ghosh, S. *et al., J. Indian Chem. Soc.*, 1928, **5**, 477 (*isol*)
Janot, M.-M. *et al., Bull. Soc. Chim. Fr.*, 1964, 2158 (*isol, ir, pmr, ms, struct*)

2-Amino-3-hydroxy-1-propanesulfonic acid A-815

Cysteinolic acid
[3687-17-0]



$$\begin{array}{c} CH_2SO_3H \\ | \\ H \blacktriangleright C \blacktriangleleft NH_2 \\ | \\ CH_2OH \end{array}$$

(*R*)–*form*

$C_3H_9NO_4S$ 155.174

Stereochem. and registry nos. are confused. Wickberg states that the L-form was isol., but his exptl. work shows clearly that it was D (i.e. *S* as it is related to D-Cysteine). CAS uses the same registry no. for L- (in 8CI) and (*S*-)(in 10CI).

(*R*)-*form*
L-form
Isol. from red alga *Polysiphonia fastigiata*. Mp 279-281° dec. $[\alpha]_D$ -6 (c, 2.0 in H_2O).

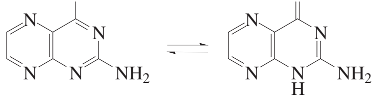
(*S*)-*form*
D-form
Isol. from brown (e.g. *Hijikia fusiforme*) and green (*Ulva pertusa*, *Enteromorpha linza*) algae. Also from diatoms, e.g. *Navicula pelliculosa* and from the starfish *Asterina pectinifera*. Mp 279-282° dec. $[\alpha]_D$ +7 (H_2O).

[15509-62-3 , 16421-58-2 , 56942-41-7]

Wickberg, B. *et al., Acta Chem. Scand.*, 1957, **11**, 506 (*isol*)
Yoneda, T. *et al., CA*, 1967, **66**, 113388p (*isol*)
Higashiura, K. *et al., J.O.C.*, 1992, **57**, 764 (*synth*)

2-Amino-4-hydroxypteridine A-816

*2-Amino-4(1*H*)-pteridinone, 9CI. 2-Amino-4-pteridinol.* ***Pterin****. Pteridoxamine*
[2236-60-4]



$C_6H_5N_5O$ 163.138

4-One-form predominates. Isol. from numerous natural sources. Yellow cryst. (HCOOH aq.). Fluoresces: violet in neutral/alkaline soln.: yellow-green in acid soln.

▶ UO3505000

8-Oxide: [42346-89-4]
$C_6H_5N_5O_2$ 179.138
Bright-yellow cryst. Mp 360°.

*2-*N-*Ac:*
$C_8H_7N_5O_2$ 205.176
Cryst. (propanol). Mp 350°. Browns at 270°.

*2-*N-*Me: 2-(Methylamino)-4(1*H*)-pteridinone, 9CI*
[13005-84-0]
$C_7H_7N_5O$ 177.165
Pale-yellow cryst. Mp 350°.

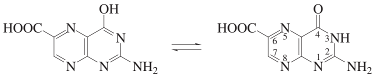
N^1-*Me: 2-Amino-1-methyl-4(1*H*)-pteridinone, 9CI*
[13005-86-2]
$C_7H_7N_5O$ 177.165
Mp 335-337° dec.

[938-42-1]

Dick, G.P.G. *et al., J.C.S.*, 1955, 1379 (*synth*)
Pfleiderer, W. *et al., Chem. Ber.*, 1960, **93**, 2015 (*synth, struct*)
Brown, D.J. *et al., J.C.S.*, 1961, 4413 (*tautom*)
Viscontini, M. *et al., Helv. Chim. Acta*, 1963, **46**, 1181 (*pmr*)
McCormack, J.J. *et al., J.O.C.*, 1964, **29**, 3370 (*synth*)
Müller, G. *et al., Helv. Chim. Acta*, 1973, **56**, 2680 (*cmr*)
Williams, V.P. *et al., J. Het. Chem.*, 1973, **10**, 827 (*ms*)
Albert, A. *et al., J.C.S. Perkin 2*, 1973, 1101 (*uv*)
Taylor, E.C. *et al., J.O.C.*, 1975, **40**, 2341 (*oxide*)
Tobias, S. *et al., Chem. Ber.*, 1985, **118**, 354 (*cmr*)

2-Amino-4-hydroxy-6-pteridinecarboxylic acid A-817

*2-Amino-1,4-dihydro-4-oxo-6-pteridinecarboxylic acid. 2-Amino-4(3*H*)-pteridinone-6-carboxylic acid. Pterin-6-carboxylic acid. Ranachrome 5*
[948-60-7]



$C_7H_5N_5O_3$ 207.148
Isol. from various biol. sources incl. human blood, sheep pineals, various amphibians, fish and soybeans. Also from the Chinese drug Jin Yu. Metab. of Pteroylglutamic acid, P-772. Cream cryst. Mp 360°.

Me ester: [31010-61-4]
$C_8H_7N_5O_3$ 221.175
Cryst. (DMF). Mp 285° dec.

*2-*N-*Ac:* [31010-65-8]
$C_9H_7N_5O_4$ 249.185
Cryst. (MeOH). Mp 210°.

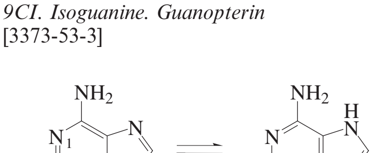
*2-*N-*Ac, Me ester:* [31010-67-0]
$C_{10}H_9N_5O_4$ 263.212
Mp 283°.

7,8-Dihydro: ***7,8-Dihydropterin-6-carboxylic acid***
$C_7H_8N_5O_3$ 210.172
Light emitter of the millipede *Luminodesmus sequoiae.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 896C (*ir*)
Baugh, C.M. *et al., J.O.C.*, 1964, **29**, 3610 (*synth*)
Pfleiderer, W. *et al., Annalen*, 1970, **741**, 64 (*synth, derivs*)
Iwanami, Y. *et al., Tet. Lett.*, 1972, 3219 (*ms*)
Nair, M.G. *et al., J.O.C.*, 1973, **38**, 2185 (*synth*)
Mengel, R. *et al., Chem. Ber.*, 1978, **111**, 3790 (*synth*)
Kohashi, M. *et al., J. Biochem. (Tokyo)*, 1980, **87**, 1581 (*isol*)
Zeitler, M. *et al., Methods Enzymol.*, 1986, **122**, 273 (*isol*)
Sato, N. *et al., J. Het. Chem.*, 1988, **25**, 1737 (*synth, derivs*)
Suga, T. *et al., J. Nat. Prod.*, 1988, **51**, 713 (*isol*)
Kuse, M. *et al., Bioorg. Med. Chem. Lett.*, 2001, **11**, 1037-1040 (*7,8-dihydro*)

6-Amino-2-hydroxypurine A-818

*6-Amino-1,3-dihydro-2*H*-purin-2-one, 9CI. Isoguanine. Guanopterin*
[3373-53-3]



$C_5H_5N_5O$ 151.127
Several tautomers possible. Aglycone from *Croton tiglium*. Isol. from the wings of the butterfly *Prioneris thestylis.* Amorph. powder. Mp 360°. pK_{a1} 4.47; pK_{a2} 9.03 (20°).

*9-(β-*D*-Arabinofuranosyl):* [38819-11-3]
$C_{10}H_{13}N_5O_5$ 283.243
Light yellow powder. Mp 269-272° dec. $[\alpha]_D^{24}$ +29.5 (c, 0.5 in H_2O).

*9-β-*D*-Ribofuranosyl:* see Isoguanosine

*1-Me: 6-Amino-1,3-dihydro-1-methyl-2*H*-purin-2-one, 9CI*
[73691-67-5]
$C_6H_7N_5O$ 165.154
Powder. Mp 300°.

*1-Me, 9-β-*D*-arabinofuranosyl: Ara-doridosine*
[77856-33-8]
$C_{11}H_{15}N_5O_5$ 297.27
Shows antiviral props. Plates (H_2O). Mp 223-225° dec. $[\alpha]_D^{24}$ +25.5 (c, 0.5 in H_2O).

*1-Me, 6-*N-*Ac:* [98933-71-2]
$C_8H_9N_5O_2$ 207.191
Cryst. (MeOH). Mp 222-223° Mp 274° dec.

1-Me, 6,9-di-Ac: [98933-69-8]
$C_{10}H_{11}N_5O_3$ 249.229
Cryst. Mp 222-223° dec. Exists as 6-imino tautomer.

*6-*N-*Me: 6-(Methylamino)-1,3-dihydro-2*H*-purin-2-one, 9CI.* ***2-Hydroxy-6-methylamino-9*H*-purine***
[24391-35-3]
$C_6H_7N_5O$ 165.154
Isol. from the blue coral NIO-156 and from the bacterium *Pseudomonas syringae*. Cytokinin. Sol. H_2O. λ_{max} 265 ; 282 (MeOH) (Berdy).

1,3-Di-Me: ***1,3-Dimethylisoguanine***. *1,3-Dimethylisoguaninium*
[191614-40-1]
$C_7H_9N_5O$ 179.181
Isol. from the sponges *Amphimedon viridis*, *Amphimedon paraviridis* and *Xestospongia exigua*. Also from *Cnemidocarpa bicornuta*. Powder; cryst. (as salt). Isol. by different groups both as the free base and as salts protonated on the imino N. λ_{max} 207 (log ϵ 4.5); 295 (log ϵ 3.9) (MeOH).

3,7-Di-Me: ***3,7-Dimethylisoguanine***
[18904-09-1]
$C_7H_9N_5O$ 179.181
Isol. from the Caribbean sponge *Agelas longissima* and *Zyzzya fuliginosa*. Sol. MeOH, butanol. λ_{max} 245 (ϵ 8500); 285 (ϵ 9900) (MeOH) (Berdy).

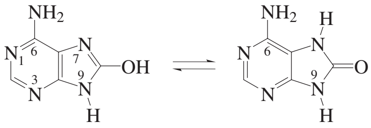
N^3,O*-Di-Me:* ***Mucronatine***†
$C_7H_9N_5O$ 179.181
Isol. from the sponge *Stryphnus mucronatus.* Solid. Mp 200-202°. Tautomeric.

*7,8-Dihydro, 6-*N-*(3-methylbutyl): 7,8-Dihydro-2-hydroxy-*N^6*-(3-methylbutyl)adenine. 7,8-Dihydro-2-hydroxy-6-(3-methylbutylamino)purine*
[188542-24-7]
$C_{10}H_{17}N_5O$ 223.277
Constit. of *Artemisia annua.*

Spies, J.R. *et al., J.A.C.S.*, 1939, **61**, 350-351 (*Isoguanine, isol*)
Purrmann, R. *et al., Annalen*, 1940, **544**, 182-190 (*Isoguanine, isol*)
Taylor, E.C. *et al., J.A.C.S.*, 1959, **81**, 2442-2448 (*Isoguanine, synth, uv*)
Veillard, A. *et al., J. Chim. Phys.*, 1962, **59**, 1056-1066 (*pmr*)
Pal, B.C. *et al., J.C.S.*, 1964, 400-405 (*ir*)
Pettit, G.R. *et al., J. Nat. Prod.*, 1976, **39**, 363-367 (*Isoguanine, isol*)
Yamazaki, A. *et al., Nucleic Acids Res.*, 1976, **3**, 251-259 (*Isoguanine, synth*)
Nachman, R.J. *et al., J.C.S. Perkin 1*, 1985, 1315-1321 (*1-Me, 1-Me-6,9-di-Ac, synth, cmr, pmr, ms, uv, ir, cryst struct*)
Farooqi, A.H.A. *et al., Phytochemistry*, 1990, **29**, 2061-2063 (*6-N-Me, isol*)
Cafieri, F. *et al., Tet. Lett.*, 1995, **36**, 7893-7896 (*3,7-Dimethylisoguanine*)
Shukla, A. *et al., J. Indian Chem. Soc.*, 1997, **74**, 59 (*Artemisia annua constit*)
Mitchell, S.S. *et al., J. Nat. Prod.*, 1997, **60**, 727-728 (*1,3-Dimethylisoguanine*)
Chehade, C.C. *et al., J. Nat. Prod.*, 1997, **60**, 729-731 (*1,3-Dimethylisoguanine*)
Do Prado, G.M.T. *et al., Acta Cryst. C*, 1999, **55**, 1585-1587 (*trihydrate, 1,3-di-Me, cryst struct*)
Bourguet-Kondracki, M.-L. *et al., Tet. Lett.*, 2001, **42**, 7257-7259 (*Mucronatine*)
Jeong, S-J. *et al., Chem. Pharm. Bull.*, 2003, **51**, 731-733 (*1,3-Dimethylisoguaninium*)
Blas, J.R. *et al., J.A.C.S.*, 2004, **126**, 154-164 (*tautom*)
Panthong, K. *et al., Acta Cryst. C*, 2006, **62**, o193-o195 (*1,3-Dimethylisoguanine, isol, cryst struct*)
Bats, J.W. *et al., Acta Cryst. E*, 2006, **62**, 2040-2042 (*cryst struct*)

6-Amino-8-hydroxypurine A-819

*6-Amino-1,7-dihydro-8*H*-purin-8-one, 9CI. 6-Amino-8-purinol, 8CI. 7,8-Dihydro-8-oxoadenine. 8-Hydroxyadenine. 8-Oxoadenine*
[21149-26-8]



$C_5H_5N_5O$ 151.127
8-Oxo-form predominates. Other tautomers are possible. Results *in vivo* from hydroxylation of DNA by OH radicals. Found in the urine of humans suffering from leukaemia. Isol. from the ascidian *Symplegma rubra* and a Thorectidae sponge. Potential cause of DNA mismatch in mutagenesis. Needles + ½H_2SO_4. Mp 300° (H_2SO_4). Unlike 2-Amino-6,8-dihydroxypurine, A-753, is not particularly mutagenic.

*6-*N-*Me:* [89073-90-5]
$C_6H_7N_5O$ 165.154
Needles (MeOH aq.). Mp >300°. λ_{max} 273 (ϵ 16900) (H_2O).

*9-Me: 6-Amino-7,9-dihydro-9-methyl-8*H*-purin-8-one, 9CI. 9-Methyl-8-oxoadenine*
[119138-92-0]
$C_6H_7N_5O$ 165.154
Isol. from a Thorectidae sponge. Prisms (H_2O). Mp 300°.

*6-*N*,9-Di-Me: 7,9-Dihydro-9-methyl-6-(methylamino)-8*H*-purin-8-one, 9CI.* N^6*,9-Dimethyl-8-oxoadenine*
[119138-91-9]
$C_7H_9N_5O$ 179.181
Needles (EtOH). Mp 300°.

N^6*-(3,5-Dibromo-4-hydroxybenzyl):*

Aplidiamine
[188348-59-6]
$C_{12}H_9Br_2N_5O_2$ 415.043
Isol. from the marine ascidian *Aplidiopsis* sp. Sol. H_2O, MeOH. Mp 241-243°. λ_{max} 221 (ε 17300); 273 (ε 15800) (MeOH/CH_2Cl_2 1:1). λ_{max} 223 (ε 19000); 290 (ε 15200) (MeOH/CH_2Cl_2/HCl). λ_{max} 223 (ε 52500); 250 (sh) ; 283 (ε 30700); 313 (sh) ; 377 (sh) (MeOH/CH_2Cl_2/NaOH).

1*H-form*

1-Me: [186391-69-5]
$C_6H_7N_5O$ 165.154
Needles +1H_2O (MeOH aq.). Mp > 300°. Various tautomers possible. λ_{max} 216 (ε 22000) (H_2O).

1,9-Di-Me: see 1,6,7,9-Tetrahydro-6-imino-1,9-dimethyl-8*H*-purin-8-one, T-194

3*H-form*

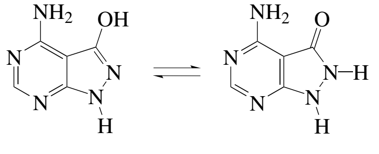
*3-Me: 6-Amino-3,7-dihydro-3-methyl-8*H*-purin-8-one. 8-Hydroxy-3-methyladenine*
[185201-03-0]
$C_6H_7N_5O$ 165.154
Needles. Mp > 300°. pK_a 4.1 (30°,H_2O). λ_{max} 232 (ε 18800) (95% EtOH).

*3,9-Di-Me: 3,6,7,9-Tetrahydro-6-imino-3,9-dimethyl-8*H*-purin-8-one, 9CI*
[198758-37-1]
[198023-18-6]
$C_7H_9N_5O$ 179.181
Plates (HCl aq.) (as hydrochloride). Mp 274-276° dec. (hydrochloride).

Robins, R.K. *et al., J.A.C.S.*, 1958, **80**, 6671-6679 (*synth, uv*)
Fujii, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2146-2150 (*Me derivs, synth, ir, uv, pmr*)
Brown, T. *et al., Chem. Br.*, 1993, **29**, 484-486 (*rev*)
Itaya, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2025-2032; 2318-2321; 1997, **45**, 1582-1588; 1867-1869 (*synth, ir, uv, pmr, bibl, Me derivs*)
Kang, H. *et al., Tet. Lett.*, 1997, **38**, 941-944 (*Aplidiamine*)
Itaya, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1297-1300 (*Aplidiamine, synth, struct*)
Lindsay, B.S. *et al., J. Nat. Prod.*, 1999, **62**, 1573-1575 (*Symplegma rubra constit*)
Madyastha, K.M. *et al., J.C.S. Perkin 1*, 1999, 677-680 (*isol*)
Makarieva, T.N. *et al., Nat. Prod. Commun.*, 2006, **1**, 711-714 (*9-Methyl-8-oxoadenine, isol*)

4-Amino-3-hydroxy-1*H*-pyrazolo[3,4-*d*]pyrimidine A-820

*4-Amino-1,2-dihydro-3*H*-pyrazolo[3,4-*d*]pyrimidin-3-one, 9CI.* ***Akalone***
[128850-54-4]

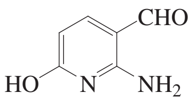


$C_5H_5N_5O$ 151.127
Prod. by the marine bacterium *Agrobacterium aurantiacum* and *Flavobacterium* sp. N-81106. Xanthine oxidase inhibitor. Powder or light green needles. Sol. bases, DMSO; poorly sol. MeOH, hexane, $CHCl_3$. Mp > 350°. λ_{max} 269 (ε 1690) (H_2O).

Anderson, J.D. *et al., J. Het. Chem.*, 1990, **27**, 439-453 (*synth*)
Japan. Pat., 1993, 93 317 070; *CA*, **120**, 189879d (*isol*)
Izumida, H. *et al., J. Mar. Biotechnol.*, 1995, **2**, 115-118 (*isol, ir, cmr, pmr*)

2-Amino-6-hydroxy-3-pyridinecarboxaldehyde A-821

2-Amino-3-formyl-6-hydroxypyridine



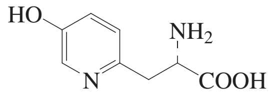
$C_6H_6N_2O_2$ 138.126

Me ether: 2-Amino-6-methoxy-3-pyridinecarboxaldehyde. 2-Amino-3-formyl-6-methoxypyridine
$C_7H_8N_2O_2$ 152.152
Alkaloid from the basidiomycete *Cortinarius umidicola*. Needles (MeOH). Mp 186-187°. λ_{max} 205 (log ε 4.32); 252 (log ε 4.38) (MeOH).

Hu, L. *et al., Z. Naturforsch., C*, 2003, **58**, 659-662 (*isol, pmr, cmr, ms*)

α-Amino-5-hydroxy-2-pyridinepropanoic acid, 9CI A-822

β-(5-Hydroxy-2-pyridyl)alanine. ***Azatyrosine****. Antibiotic SF 1346. SF 1346*



$C_8H_{10}N_2O_3$ 182.179
Amino acid antibiotic.

(*S*)*-form* [58525-82-9]
Isol. from *Streptomyces chibaensis*. Antiviral, antitumour, antibacterial and antineoplastic agent. Also shows antiinflammatory activity. Cryst. (H_2O). Sol. H_2O, MeOH, butanol-H_2O, bases; fairly sol. EtOH; poorly sol. Me_2CO, hexane. Mp 262-263° dec. $[\alpha]_D^{25}$ -33 (c, 1.0 in H_2O). $[\alpha]_D$ +55 (c, 1.1 in 1*M* HCl). λ_{max} 219 (E1%/1cm 330); 280 (E1%/1cm 140); 320 (E1%/1cm 15) (H_2O) (Berdy). λ_{max} 228 (E1%/1cm 175); 289 (E1%/1cm 235) (HCl) (Berdy). λ_{max} 241 (E1%/1cm 445); 302 (E1%/1cm 165) (NaOH) (Berdy).

Hydrochloride (1:3):
Hygroscopic foam + 2½H_2O. $[\alpha]_D^{25}$ +28 (c, 0.06 in 1*M* HCl).

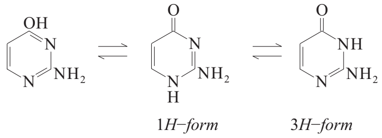
Me ester: [58485-16-8]
Cryst. (as hydrochloride). Mp 224-225° dec. (hydrochloride). $[\alpha]_D^{20}$ +38 (c, 1.0 in H_2O).

(±)*-form* [943-82-8]
Prisms (H_2O). Mp 272-273° dec.

Inouye, S. *et al., Chem. Pharm. Bull.*, 1975, **23**, 2669 (*isol*)
Harris, R.L.N. *et al., Aust. J. Chem.*, 1977, **30**, 649 (*isol*)
Ger. Pat., 1978, 2 823 346; *CA*, **90**, 133025s (*synth, props*)
Fukuyasu, H. *et al., CA*, 1984, **101**, 48223 (*props*)
Izawa, M. *et al., Cancer Res.*, 1992, **52**, 1628-1630 (*pharmacol*)
Schow, S.R. *et al., J.O.C.*, 1994, **59**, 6850 (*synth*)
Ye, B. *et al., J.O.C.*, 1995, **60**, 2640 (*synth, ir, pmr*)
Coper, M.S. *et al., Bioorg. Med. Chem. Lett.*, 1996, **6**, 2613 (*synth*)
Myers, A.G. *et al., J.O.C.*, 1996, **61**, 813 (***synth, ir, pmr, bibl***)
Monden, Y. *et al., Ann. N.Y. Acad. Sci.*, 1999, **886**, 109-121 (*rev, activity*)

2-Amino-4-hydroxypyrimidine A-823

*2-Amino-4(1*H*)-pyrimidinone, 9CI. 2-Amino-4-pyrimidinol. Isocytosine*
[108-53-2]



$C_4H_5N_3O$ 111.103
NH-forms predominate. Prisms (H_2O). Mp 280° dec. pK_{a1} 3.91; pK_{a2} 9.54 (25°).

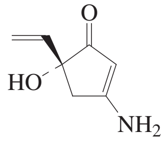
1*H-form*

*1-β-*D*-Ribopyranosyl:* ***Isocytidine***
[489-59-8]
$C_9H_{13}N_3O_5$ 243.219
Isol. from a strain of *Penicillium brevicompactum*. Glass. λ_{max} 256 nm, λ_{min} 240 nm (H_2O, pH1).

Lis, A.W. *et al., Biochim. Biophys. Acta*, 1962, **61**, 250 (*Isocytidine*)

3-Amino-5-hydroxy-5-vinyl-2-cyclopenten-1-one A-824

3-Amino-5-ethenyl-5-hydroxy-2-cyclopenten-1-one, 9CI



$C_7H_9NO_2$ 139.154
Incorrect struct. given in CAS.

(*R*)*-form*
Myrothenone B
[878633-73-9]
[858126-05-3]
Prod. by *Streptomyces* sp. GT-20026114 obt. from the mangrove plant *Aegiceras comiculatum* and from a marine-derived fungus *Myrothecium* sp. Yellowish oil. $[\alpha]_D^{20}$ +127.1 (c, 1.54 in MeOH). $[\alpha]_D^{20}$ +35 (c, 0.6 in MeOH). λ_{max} 270 (MeOH). λ_{max} 203 (log ε 3.7); 268 (log ε 4) (MeOH).

N-Formyl: ***Myrothenone A***
$C_8H_9NO_3$ 167.164
Prod. by *Myrothecium* sp. Tyrosinase inhibitor. Oil. $[\alpha]_D^{20}$ +61 (c, 0.6 in MeOH). λ_{max} 203 (log ε 3.7); 272 (log ε 4.2) (MeOH).

N-*Methoxycarbonyl:* [878633-74-0]
$C_9H_{11}NO_4$ 197.19
Prod. by *Streptomyces* sp. GT-20026114. Yellowish oil. $[\alpha]^{20}_{D}$ +67.6 (c, 1.16 in MeOH). λ_{max} 261 (MeOH).

N,N-*Di-Me:* ***3-(Dimethylamino)-5-hydroxy-5-vinyl-2-cyclopenten-1-one***. *3-(Dimethylamino)-5-ethenyl-5-hydroxy-2-cyclopenten-1-one*
[179422-20-9]
Isol. from *Trichoderma koningii*. Amorph. powder. Sol. H_2O, MeOH, $CHCl_3$, DMSO; fairly sol. Me_2CO, MeCN, EtOAc; poorly sol. hexane. Mp 137-139°. $[\alpha]^{20}_{D}$ +69.3 (c, 0.2 in H_2O). Biol. inactive. λ_{max} 280 (ϵ 30000) (MeOH).

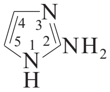
N-*[2-(4-Hydroxyphenyl)ethyl]:* [878633-75-1]
$C_{15}H_{17}NO_3$ 259.304
Prod. by *Streptomyces* sp. GT-20026114. Yellowish oil. $[\alpha]^{20}_{D}$ +59.3 (c, 1.73 in MeOH). λ_{max} 232 (MeOH).

2-Bromo: 3-Amino-2-bromo-5-hydroxy-5-vinyl-2-cyclopenten-1-one. ***2-Bromomyrothenone B***
[929276-07-3]
$C_7H_8BrNO_2$ 218.05
Prod. by a marine-derived *Botrytis* sp. Red oil. $[\alpha]^{20}_{D}$ +61 (c, 0.9 in MeOH). λ_{max} 210 (log ϵ 3.7); 277 (log ϵ 4.2) (MeOH).

Mukhopadhyay, T. *et al., J. Antibiot.*, 1996, **49**, 210-211 (*N,N-di-Me*)
Li, X. *et al., Chem. Pharm. Bull.*, 2005, **53**, 453-455 (*Myrothenones A,B*)
Lin, W. *et al., J. Antibiot.*, 2005, **58**, 594-598 (*isol, cd, pmr, cmr, ms*)
Li, X. *et al., J. Nat. Prod.*, 2007, **70**, 307-309 (*2-Bromomyrothenone B*)

2-Aminoimidazole, 8CI A-825

*1*H*-Imidazol-2-amine, 9CI. 2-Aminoglyoxaline*
[7720-39-0]



$C_3H_5N_3$ 83.093
Isol. from the sponges *Halichondria* sp. and *Reniera cratera*. Also occurs in the seeds of the legume *Mundulea sericea*, and has been shown to be a precursor of the antibiotic 2-Nitroimidazole, N-250 in *Streptomyces eurocidicus*.

Hydrochloride: [57575-96-9]
Mp 152°. Hygroscopic.

Nitrate: Mp 135-136°.

Sulfate (2:1): [1450-93-7]
[42383-61-9]
Mp 270° dec.

Picrate: Mp 236°.

*2-*N*-Ac: 2-Acetamidoimidazole*
[52737-49-2]
$C_5H_7N_3O$ 125.13
Mp 285° (270-275°) dec.

1-Me: [6646-51-1]
$C_4H_7N_3$ 97.119
Prismatic needles (EtOH/EtOAc) (as hydrochloride). Mp 84° (hydrochloride).

[1450-94-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 614D (*ir*)
Lawson, A. *et al., J.C.S.*, 1956, 307 (*synth*)
Seki, Y. *et al., J. Biochem. (Tokyo)*, 1970, **67**, 389 (*isol, ir, pmr*)
Cimino, G. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1974, **47**, 895 (*isol, uv, pmr, ms*)
Fellows, L.E. *et al., Phytochemistry*, 1977, **16**, 1399 (*isol, pmr, ms*)
Kirk, K.L. *et al., J.O.C.*, 1978, **43**, 4381-4383 (*synth, pmr*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1984, 124-125; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 126-127 (*isol, Halichondria*)
Weinmann, H. *et al., Tet. Lett.*, 2002, **43**, 593-595 (*synth, ir, pmr*)
Yano, S. *et al., Chem. Pharm. Bull.*, 2004, **12**, 3443-3450 (*1-Me, synth, pmr*)

4(5)-Aminoimidazole A-826

*1*H*-Imidazol-4-amine. 4-Aminoglyoxaline*
[4919-03-3]
$C_3H_5N_3$ 83.093
Present in biotin-restricted yeast. Mp 184° (as hydrochloride).

N^4*-Ac:* [51741-72-1]
$C_5H_7N_3O$ 125.13
Cryst. (dioxan). Sol. H_2O. Mp 226°.

N^4*-Ac, picrate:* Mp 208°.

1H-form

*1-Benzyl: 4-Amino-1-benzyl-1*H*-imidazole*
[53594-77-7]
$C_{10}H_{11}N_3$ 173.217
Cryst, (MeCN) (as hydrochloride). Mp 179-182° (hydrochloride). CAS no. refers to hydrochloride.

1-Benzyl, N^4*-Ac:* [7524-03-0]
$C_{12}H_{13}N_3O$ 215.254
Cryst. (EtOAc). Mp 168-168.8°.

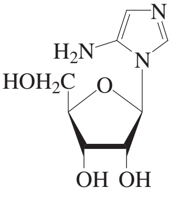
3H-form

*3-Me: 5-Amino-1-methyl-1*H*-imidazole*
[66787-75-5]
$C_4H_7N_3$ 97.119
Purple solid. Mp 107-109°.

Hunter, G. *et al., Can. J. Res., Sect. B*, 1941, **19**, 296; *CA*, **36**, 1321 (*synth, N-Ac*)
Whitaker, J.M. *et al., Arch. Biochem. Biophys.*, 1962, **96**, 541 (*isol*)
Coburn, M.D. *et al., J. Het. Chem.*, 1970, **7**, 1391-1393 (*synth*)
Buchman, R. *et al., J. Med. Chem.*, 1974, **17**, 1168-1171 (*N-benzyl derivs*)
Al-Shaar, A.H.M. *et al., J.C.S. Perkin 1*, 1992, 2779 (*3-Me*)

5-Aminoimidazole riboside A-827

*1-β-*D*-Ribofuranosyl-1*H*-imidazol-5-amine, 9CI*
[30597-39-8]

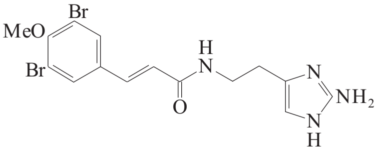


$C_8H_{13}N_3O_4$ 215.208
Prod. by *Escherichia coli* strain K-12. Hygroscopic pale grey solid. Mp 92-94°. λ_{max} 300 (no solvent reported).

5′-Phosphate: 5-Aminoimidazole ribonucleotide. AIR
[25635-88-5]
$C_8H_{14}N_3O_7P$ 295.188
Intermed. in biosynth. of purine ribonucleotides. Precursor of thiamine in *Escherichia coli*. Solid.

Love, S.H. *et al., Biochim. Biophys. Acta*, 1959, **35**, 367 (*isol*)
Schrimsher, J.L. *et al., Biochemistry*, 1986, **25**, 4356-4365 (*synth, pmr, cmr*)
Bhat, B. *et al., J.A.C.S.*, 1990, **112**, 4891-4897 (*synth, pmr*)
Firestine, S.M. *et al., Biochemistry*, 1994, **33**, 11917-11926 (*synth, ir, pmr, cmr*)
Humphries, M.J. *et al., Synthesis*, 1999, 985-992 (*synth, pmr*)

N-[2-(2-Amino-1*H*-imidazol-4-yl)ethyl]-3-(3,5-dibromo-4-methoxyphenyl)-2-propenamide, 9CI A-828



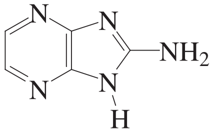
$C_{15}H_{16}Br_2N_4O_2$ 444.125

(E)-form [160491-72-5]
Metab. from the Caribbean sponge *Verongula* sp. Amorph. solid (as trifluoroacetate). CAS no. refers to trifluoroacetate.

Ciminiello, P. *et al., J. Nat. Prod.*, 1994, **57**, 1564 (*isol, uv, ir, pmr, cmr, struct*)

2-Amino-1*H*-imidazo[4,5-*b*]pyrazine A-829

*1*H*-Imidazo[4,5-*b*]pyrazin-2-amine.* ***Zarzissine***

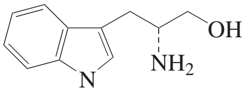


$C_5H_5N_5$ 135.128
Struct. of Zarzissine revised in 2001. Alkaloid from the Mediterranean sponge *Anchinoe paupertas*. Cytotoxic. Active against *Candida*, bacteria and some tumour lines. Cryst. (H_2O or MeOH). Mp > 300° dec. λ_{max} 217 (sh) ; 244 (log ϵ 3.3); 318 (log ϵ 4.03) (MeOH). λ_{max} 206 (log ϵ 4.31); 230 (sh) ; 282 (sh) ; 326 (log ϵ 5.39) (MeOH/NaOH).

Bouaicha, N. *et al., J. Nat. Prod.*, 1994, **57**, 1455 (*isol*)
Wan, Z.K. *et al., Tetrahedron*, 2001, **57**, 5497-5507 (*synth, uv, pmr, cmr*)

2-Amino-3-(3-indolyl)-1-propanol A-830

*β-Amino-1*H*-indole-3-propanol, 9CI. Tryptophanol*
[526-53-4]


(*R*)-form

$C_{11}H_{14}N_2O$ 190.244
▶NM1320000

(*R*)-*form*
D-form
[52485-52-6]
Cryst. (EtOAc). Mp 80-81°. $[\alpha]_D^{25}$ +20.9 (c, 1 in MeOH).
Oxalate salt (1:1): [58889-66-0]
Mp 202-203°. $[\alpha]_D^{20}$ +22.1 (c, 1.02 in H_2O).

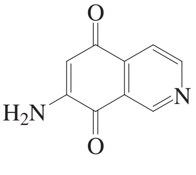
(*S*)-*form*
L-form
[2899-29-8]
Cryst. (EtOAc). Mp 84-85°. $[\alpha]_D^{25}$ -20.5 (c, 1 in MeOH).
Oxalate salt (1:1): [2899-30-1]
Mp 203-205°. $[\alpha]_D^{20}$ -22.4 (c, 1.03 in H_2O).
N-*Ac:* **N-*Acetyltryptophanol***
$C_{13}H_{16}N_2O_2$ 232.282
Prod. by *Streptomyces pleomorphus* (strain YIM33176). Amorph. powder. $[\alpha]_D^{25}$ +27 (c, 1.2 in $CHCl_3$). λ_{max} 221 (log ϵ 4.49); 281 (log ϵ 3.77) (no solvent reported).

(±)-*form* [154-09-6]
Cryst. (C_6H_6). Mp 85-86°.
Hydrochloride: [25825-57-4]
Cryst. (EtOH/Et_2O). Mp 178-179°.

Hellmann, H. *et al., Chem. Ber.*, 1958, **91**, 2290 (*synth*)
Ito, A. *et al., Chem. Pharm. Bull.*, 1975, **23**, 3106 (*synth*)
Repke, D.B. *et al., J. Het. Chem.*, 1976, **13**, 775 (*synth, pmr*)
Hvidt, T. *et al., Can. J. Chem.*, 1988, **66**, 779 (*synth, pmr, cmr*)
Li, Y.Q. *et al., Chin. Chem. Lett.*, 2005, **16**, 613-615 (*N-Acetyltryptophanol*)

7-Amino-5,8-isoquinolinedione A-831

7-Amino-5,8-isoquinolinequinone

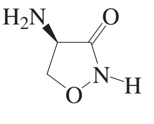


$C_9H_6N_2O_2$ 174.159
N^7-*Me: 7-(Methylamino)-5,8-isoquinolinedione, 9CI.* ***Caulibugulone A***
[662167-15-9]
$C_{10}H_8N_2O_2$ 188.185
Alkaloid from the marine bryozoan *Caulibugula intermis.* Cytotoxic. Dark red solid. λ_{max} 237 (log ϵ 4.24); 268 (log ϵ 4.1); 451 (log ϵ 3.61) (MeOH).
N^7-*(2-Hydroxyethyl): 7-[(2-Hydroxyethyl)amino]-5,8-isoquinolinedione.* ***Caulibugulone D***
[662167-18-2]
$C_{11}H_{10}N_2O_3$ 218.212
Alkaloid from *Caulibugula intermis.* Cytotoxic. Dark orange solid. λ_{max} 273 (log ϵ 3.95); 450 (log ϵ 3.35) (MeOH).
N^7-*Me, 5-imine:* ***Caulibugulone E***
[662167-19-3]
$C_{10}H_9N_3O$ 187.201
Alkaloid from *Caulibugula intermis.* Cytotoxic. Dark orange solid (as TFA salt). λ_{max} 213 (log ϵ 3.71); 245 (log ϵ 3.75); 441 (log ϵ 3.09) (MeOH) (TFA salt).
N^7-*Me, 5-(2-hydroxyethyl)imide:* ***Caulibugulone F***
[662167-20-6]
$C_{12}H_{13}N_3O_2$ 231.254
Alkaloid from *Caulibugula intermis.* Cytotoxic. Dark orange solid (as TFA salt). λ_{max} 215 (log ϵ 3.79); 245 (log ϵ 3.75); 440 (log ϵ 3.16) (MeOH) (TFA salt).
6-Chloro, N^7-*Me: 6-Chloro-7-(methylamino)-5,8-isoquinolinedione.* ***Caulibugulone B***
[662167-17-1]
$C_{10}H_7ClN_2O_2$ 222.63
Alkaloid from *Caulibugula intermis.* Cytotoxic. Dark red solid. λ_{max} 251 (log ϵ 4.03); 274 (log ϵ 3.97); 475 (log ϵ 3.36) (MeOH).
6-Bromo, N^7-*Me: 6-Bromo-7-(methylamino)-5,8-isoquinolinedione.* ***Caulibugulone C***
[662167-16-0]
$C_{10}H_7BrN_2O_2$ 267.082
Alkaloid from *Caulibugula intermis.* Cytotoxic. Dark red solid. λ_{max} 254 (log ϵ 4); 272 (log ϵ 3.97); 474 (log ϵ 3.49) (MeOH).

Milanowski, D.J. *et al., J. Nat. Prod.*, 2004, **67**, 70-73 (*Caulibugulones, isol, pmr, cmr*)
Wipf, P. *et al., Org. Biomol. Chem.*, 2004, **2**, 2173-2174 (*synth, activity*)
Alagille, D. *et al., Tet. Lett.*, 2004, **45**, 6179-6181 (*synth*)

4-Amino-3-isoxazolidinone, 9CI, 8CI A-832

Cycloserine, BAN, INN, USAN. *Cyclomycin. Closina. Micoserina. Farmiserina. Orientomycin. Oxymycin. Antibiotic 106-7. Antibiotic 5915. Antibiotic 8217. Antibiotic 17452. Antibiotic E 733A. Antibiotic I 1431. Antibiotic K 300. Antibiotic NJ 21. Antibiotic PA 94. Antibiotic Ro 1-9213. Oxamycin. Seromycin. Orientmycin. Many other names*
[4834-58-6]


(*R*)-form

$C_3H_6N_2O_2$ 102.093
λ_{max} 226 (ϵ 4140) (H_2O) (Derep).

(*R*)-*form* [68-41-7]
Prod. by *Streptomyces garyphalus, Streptomyces orchidaceus, Streptomyces lavendulae* and *Streptomyces nagasakiensis.* Shows antibiotic activity primarily against mycobacteria. Tuberculostatic. Cryst. Sol. H_2O, alkalis. Mp 155-156° dec. $[\alpha]_D^{23}$ +116 (c, 1.17 in H_2O). Of limited clinical use due to toxicity.
▶CNS adverse effects reported when used therapeutically. LD_{50} (mus, orl) 5290 mg/kg. NY2975000
N-*Ac:*
$C_5H_8N_2O_3$ 144.13
Needles. Mp 179-180°.
N,N′-*Di-Ac:*
$C_7H_{10}N_2O_4$ 186.167
Chunky needles (Me_2CO). Mp 121-122°.

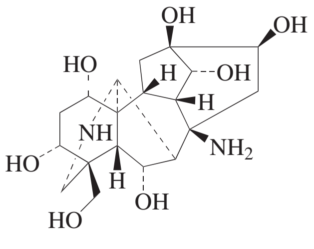
(*S*)-*form*
Levcycloserine, INN, USAN
[339-72-0]
Enzyme inhibitor used in the treatment of Gaucher's disease. Mp 146° dec. $[\alpha]_D^{20}$ -104 (c, 1 in H_2O).
▶NY2976000

(±)-*form* [68-39-3]
Mp 137-140°.
▶NY2974900

[339-72-0]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 678B; 678C; 678D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 810A; 810D; 811A (*ir*)
Harned, R.L. *et al., Antibiot. Chemother. (Washington, D.C.)*, 1955, **5**, 204 (*struct*)
Stammer, C.H. *et al., J.A.C.S.*, 1955, **77**, 2344; 2345; 2346; 1957, **79**, 3236 (*struct, synth, isol, resoln*)
Neuhaus, F.C. *et al., Antibiotics (N.Y.)*, 1967, **1**, 40 (*rev*)
Milne, G.W.A. *et al., Tetrahedron*, 1967, **23**, 65 (*nmr, ms*)
Lamb, J.W. *et al., Anal. Profiles Drug Subst.*, 1972, **1**, 53 (*rev, synth, anal*)
O'Brien, P. *et al., Met. Ions Biol. Syst.*, 1985, **19**, 295 (*rev, pharmacol*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 107 (*synonyms*)
El-Obeid, H.A. *et al., Anal. Profiles Drug Subst.*, 1989, **18**, 567 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 156
Hofmann, S.G. *et al., CNS Drug Rev.*, 2006, **12**, 208-217 (*rev, pharmacol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CQH000

8-Amino-4-methylaconitane-1,3,6,13,14,16,18-heptol A-833



$C_{19}H_{30}N_2O_7$ 398.455

(1α,3α,5β,6α,14α,16β)-*form*

O^1,O^6,O^{16},O^{18}-*Tetra-Me,* N-*Et:* ***Hemsleyatine***

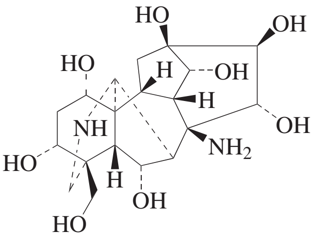
[618456-73-8]

$C_{25}H_{42}N_2O_7$ 482.616

Alkaloid from the roots of *Aconitum hemsleyanum*. Amorph. powder. Mp 89-90°. $[\alpha]_D$ +36.5 (c, 0.55 in $CHCl_3$).

Zhou, X.L. *et al., Chem. Pharm. Bull.*, 2003, **51**, 592-594 (*Hemsleyatine*)

8-Amino-4-methylaconitane-1,3,6,13,14,15,16,18-octol A-834



$C_{19}H_{30}N_2O_8$ 414.455

(1α,3α,5β,6α,14α,15α,16β)-*form*

O^1,O^6,O^{16},O^{18}-*Tetra-Me,* N-*Et:* ***Lasianine***

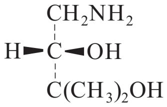
[799782-01-7]

$C_{25}H_{42}N_2O_8$ 498.615

Alkaloid from the roots of *Aconitum nagarum* var. *lasiandrum*. Needles. Mp 134-136°. $[\alpha]_D$ +12.9 (c, 0.4 in MeOH).

Ji, H. *et al., Heterocycles*, 2004, **63**, 2363-2370 (*isol, pmr, cmr*)

1-Amino-3-methyl-2,3-butanediol A-835



$$\begin{array}{c} CH_2NH_2 \\ H\blacktriangleright C\blacktriangleleft OH \\ C(CH_3)_2OH \end{array}$$

$C_5H_{13}NO_2$ 119.163

(*S*)-*form*

N-*Ac:* N-*(2,3-Dihydroxy-3-methylbutyl)acetamide, 9CI*

[81892-89-9]

$C_7H_{15}NO_3$ 161.2

Isol. from *Verbesina encelioides*. $[\alpha]_D^{25}$ -20.7 (c, 0.15 in $CHCl_3$).

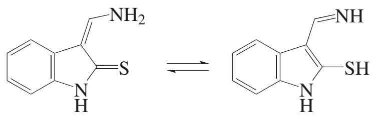
Eichholzer, J.V. *et al., Phytochemistry*, 1982, **21**, 97 (*isol, struct, synth*)

Eichholzer, J.V. *et al., Aust. J. Chem.*, 1986, **39**, 1907 (*synth, abs config, pmr, cmr*)

3-(Aminomethylene)-1,3-dihydro-2*H*-indole-2-thione A-836

3-Aminomethyleneindole-2-thione

[212390-47-1]



$C_9H_8N_2S$ 176.242

Intermed. in the detoxification of the phytoalexins Cyclobrassinin, C-842 and Brassinin, B-284 by the fungus *Leptosphaeria maculans/Phoma lingam*. Mp 197-200°.

Pedras, M.S.C. *et al., Chem. Comm.*, 1998, 1565-1566 (*synth, pmr, cmr*)

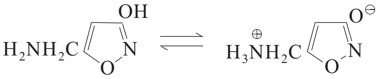
Pedras, M.S.C. *et al., J. Agric. Food Chem.*, 1999, **47**, 1196-1202 (*isol, synth, pmr, cmr*)

Pedras, M.S.C. *et al., Org. Biomol. Chem.*, 2005, **3**, 2002-2007 (*isol*)

5-(Aminomethyl)-3(2*H*)-isoxazolone, 9CI A-837

Pantherine. *Agarin. Muscimol. Pyroibotenic acid. β-Toxin*

[2763-96-4]



$C_4H_6N_2O_2$ 114.104

Exists as betaine in solid phase. Constit. of fly agaric (*Amanita muscaria*). GABA$_A$ agonist. Used in neurochemical research. Insecticide against flies. Cryst. (EtOH). Sol. H_2O. Mp 174-176° dec. λ_{max} 212 (ε 9700) (H_2O) (Berdy). λ_{max} 220 (ε 7500) (pH 12 buffer) (Berdy). λ_{max} 212 (ε 8700) (pH 2 buffer) (Berdy).

▶ LD_{50} (rat, orl) 45 mg/kg. NY3325000

Nakamura, N. *et al., Chem. Pharm. Bull.*, 1971, **19**, 46 (*synth*)

Brehm, C. *et al., Acta Chem. Scand.*, 1972, **26**, 1298 (*cryst struct*)

Krogsgaard-Larsen, P. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 281; 1981, **35**, 311 (*synth, pharmacol*)

McCarry, B.E. *et al., Tet. Lett.*, 1981, 5153 (*synth*)

Konda, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1083 (*ir, pmr, cmr, struct, synth, bibl*)

Chiarino, D. *et al., Tet. Lett.*, 1986, **27**, 3181 (*synth*)

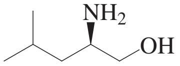
Pevarello, P. *et al., Synth. Commun.*, 1992, **22**, 1939 (*synth*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKT750

2-Amino-4-methyl-1-pentanol, 9CI A-838

2-Amino-1-hydroxy-4-methylpentane. Leucinol

[502-32-9]



(*R*)-*form*

$C_6H_{15}NO$ 117.191

(*R*)-*form*

D-form

[53448-09-2]

Bp_{11} 98-99°.

Oxalate: Mp 216°. $[\alpha]_D^{20}$ -7.

(*S*)-*form*

L-form

[7533-40-6]

[14438-11-0] Bp_{11} 98-99°. $[\alpha]_D^{17}$ +4.15 (EtOH).

N-tert-*Butyloxycarbonyl:* [82010-31-9]

$C_{11}H_{23}NO_3$ 217.308

Oil. Bp_5 141°. $[\alpha]_D^{20}$ -28.36 (c, 0.95 in $CHCl_3$).

N-*Benzyl:* [10249-88-4]

$C_{13}H_{21}NO$ 207.315

Cryst. Mp 70°. $[\alpha]_D^{20}$ +31 (c, 1.0 in $CHCl_3$).

(±)-*form* [16369-17-8] Sol. H_2O, EtOH, spar. sol. Et_2O. Bp 198-200°.

Hydrochloride: Mp 161-162°.

(ξ)-*form*

N-*Ac:* N-*[1-(Hydroxymethyl)-3-methylbutyl]acetamide, 9CI.* N-*[2-(1-Hydroxy-4-methylpentyl)]acetamide*

[150206-13-6]

$C_8H_{17}NO_2$ 159.228

Prod. by *Streptomyces globisporus* and *Streptomyces griseus.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 337A (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 541C (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 426D; 427A (*ir*)

Karrer, W. *et al., Helv. Chim. Acta*, 1921, **4**, 90; 1948, **31**, 1617 (*synth, abs config*)

Enz, W. *et al., Helv. Chim. Acta*, 1946, **29**, 1048 (*synth, use*)

Adkins, H. *et al., J.A.C.S.*, 1947, **69**, 3039 (*synth*)

Dillon, J. *et al., J.A.C.S.*, 1975, **97**, 5409; 5825 (*config*)

Jizba, J. *et al., Coll. Czech. Chem. Comm.*, 1993, **58**, 1452-1456 (*N-Ac, isol, pmr, cmr, ms*)

Ibuka, T. *et al., J.O.C.*, 1997, **62**, 999-1015 (*N-tert-butoxycarbonyl, synth, ir, pmr*)

Braüner-Osborne, H. *et al., Org. Biomol. Chem.*, 2005, **3**, 3926-3936 (*N-benzyl*)

4-Amino-4-methyl-2-pentanone, 9CI A-839

Diacetonamine

[625-04-7]

$(H_3C)_2C(NH_2)CH_2COCH_3$

$C_6H_{13}NO$ 115.175

Isol. from *Genista hystrix* subspecies. Also isol. as a salt from *Temnopleurus hardwickii*. Mod. sol. H_2O. Bp 178-181° $Bp_{0.2}$ 25°. *G.* isolates stated to be prob. as artifacts.

Oxime: [69151-99-1]

$C_6H_{14}N_2O$ 130.189

Needles. Mp 58°. Bp_{14} 130°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 460A (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 659B (*nmr*)

Haeseler, P.R. *et al., J.A.C.S.*, 1925, **47**, 1195 (*synth*)

Org. Synth., Coll. Vol., 1, 1932, 191 (*synth*)

Smith, M.E. *et al., J.A.C.S.*, 1938, **60**, 408 (*synth*)

U.S. Pat., 1950, 2 497 548; *CA*, **44**, 4494 (*synth*)

Steinegger, E. *et al., Pharm. Acta Helv.*, 1976, **51**, 172; 203 (*isol, Genista*)

Chen, L. *et al., J. Nat. Prod.*, 2006, **69**, 1787-1789 (*isol, Temnopleurus*)

1-Amino-2-methyl-2-propanol, 9CI A-840

*Amino-*tert*-butyl alcohol. 2-Hydroxyisobutylamine. Aminotrimethylcarbinol*
[2854-16-2]
$(H_3C)_2C(OH)CH_2NH_2$

$C_4H_{11}NO$ 89.137
Component of phospholipids of *Neurospora crassa*. d_{20}^{20} 0.93. Bp 151° Bp_{20} 81°. n_D^{18} 1.4460.

▶ UA6125000

Hydrochloride: [30533-50-7]
Hygroscopic cryst. Mp 62-65°.

N-*Benzoyl:* [33561-46-5]
$C_{11}H_{15}NO_2$ 193.245
Mp 108°.

N,N-*Di-Me: 1-(Dimethylamino)-2-methyl-2-propanol*
[14123-48-9]
$C_6H_{15}NO$ 117.191
Aggregation pheromone of cockroach *Blattella germanica*. Liq. Bp_{48} 60°.

N-*(2,4-Dinitrophenyl):*
Yellow-orange cryst. (C_6H_6/petrol). Mp 107-108°.

[119330-21-1]

Krassusky, K. *et al., C. R. Hebd. Seances Acad. Sci.*, 1908, **146**, 238 (*synth*)
Cairn, T.L. *et al., J.A.C.S.*, 1941, **63**, 1034 (*synth*)
Vanderwerf, C.A. *et al., J.A.C.S.*, 1954, **76**, 1231 (*synth*)
Ellman, G.L. *et al., J.A.C.S.*, 1954, **76**, 4028 (*isol*)
Pfleiderer, W. *et al., Chem. Ber.*, 1966, **99**, 3008 (*synth*)
Magnet, M. *et al., Bull. Soc. Chim. Fr.*, 1978, 539; 550 (*synth*)
Sakuma, M. *et al., Appl. Entomol. Zool.*, 1990, **25**, 355 (*N-di-Me, isol*)
Rai, B.L. *et al., J. Med. Chem.*, 1998, **41**, 3347-3359 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ALB250

2-(Aminomethyl)-2-propenoic acid, 9CI A-841

3-Amino-2-methylenepropanoic acid. α-Methylene-β-alanine
[4452-16-8]
$H_2C{=}C(COOH)CH_2NH_2$

$C_4H_7NO_2$ 101.105
Toxic amino acid from the sponge *Fasciospongia cavernosa* and other sponges. Also prod. by a *Streptomyces* sp. Shows herbicidal props. Sol. H_2O.

Hydrochloride: [75509-28-3]
Cryst. (MeOH/Me_2CO). Mp 153-154°.

Me ester: [87375-90-4]
$C_5H_9NO_2$ 115.132
From *Fasciospongia cavernosa*. Mp 107-108° (as hydrochloride).

N-*Tetradecanoyl:* [70290-27-6]
$C_{18}H_{33}NO_3$ 311.464
Isol. from *Spongia* cf. *zimocca*.

N-*Pentadecanoyl:* [70290-28-7]
$C_{19}H_{35}NO_3$ 325.49
Isol. from *Spongia* cf. *zimocca*.

N-*Hexadecanoyl:* [70290-29-8]
$C_{20}H_{37}NO_3$ 339.517
Isol. from *Spongia* cf. *zimocca*.

N-*Tetradecanoyl, Me ester:* [70290-25-4]
$C_{19}H_{35}NO_3$ 325.49
Isol. from *Fasciospongia cavernosa* and *Spongia* cf. *zimocca*.

N-*Pentadecanoyl, Me ester:* [70290-26-5]
$C_{20}H_{37}NO_3$ 339.517
Isol. from *Fasciospongia cavernosa* and *Spongia* cf. *zimocca*.

N-*Hexadecanoyl, Me ester:* [52634-29-4]
$C_{21}H_{39}NO_3$ 353.544
Isol. from *Fasciospongia cavernosa*, a *Hippospongia* sp. and *Spongia* cf. *zimocca*.

N-*(14-Methylpentadecanoyl), Me ester:* ***Hurghamide A***
$C_{21}H_{39}NO_3$ 353.544
Isol. from a *Hippospongia* sp. Wax.

N-*(15-Methylhexadecanoyl), Me ester:* ***Hurghamide B***
$C_{22}H_{41}NO_3$ 367.571
Isol. from a *Hippospongia* sp. Wax.

N-*(Methylhexadecanoyl), Me ester:* ***Hurghamide C***
$C_{22}H_{41}NO_3$ 367.571
Isol. from a *Hippospongia* sp. Wax. Posn. of methyl on *N*-acyl group not determined.

N-*Heptadecanoyl, Me ester:* [52634-30-7]
$C_{22}H_{41}NO_3$ 367.571
Isol. from *Fasciospongia cavernosa* and a *Hippospongia* sp.

N-*(13-Octadecenoyl), Me ester:* ***Hurghamide D***
$C_{23}H_{41}NO_3$ 379.582
Isol. from a *Hippospongia* sp.

N-*Octadecanoyl, Me ester:* [52634-31-8]
$C_{23}H_{43}NO_3$ 381.598
Isol. from *Fasciospongia cavernosa.*

N-*Nonadecanoyl, Me ester:* [52634-32-9]
$C_{24}H_{45}NO_3$ 395.624
Isol. from *Fasciospongia cavernosa.*

N-*Eicosanoyl, Me ester:* [52634-33-0]
$C_{25}H_{47}NO_3$ 409.651
Isol. from *Fasciospongia cavernosa.*

N-*(2-Oxotetradecanoyl), Me ester:*
[70290-19-6]
$C_{19}H_{33}NO_4$ 339.474
Isol. from *Spongia* cf. *zimocca* and *Sinularia dissecta*.

N-*(2-Oxopentadecanoyl), Me ester:*
[70290-20-9]
$C_{20}H_{35}NO_4$ 353.501
Isol. from *Spongia* cf. *zimocca* and *Sinularia dissecta*.

N-*(2-Oxohexadecanoyl), Me ester:*
[70290-21-0]
$C_{21}H_{37}NO_4$ 367.528
Isol. from *Spongia* cf. *zimocca*.

N-*(2-Hydroxytetradecanoyl), Me ester:*
[70290-22-1]
$C_{19}H_{35}NO_4$ 341.49
Isol. from *Spongia* cf. *zimocca*.

N-*(2-Hydroxypentadecanoyl), Me ester:*
[70290-23-2]
$C_{20}H_{37}NO_4$ 355.517
Isol. from *Spongia* cf. *zimocca*.

N-*(2-Hydroxyhexadecanoyl), Me ester:*
[70290-24-3]
$C_{21}H_{39}NO_4$ 369.543
Isol. from *Spongia* cf. *zimocca*.

N-*(2-Acetoxy-2-tetradecenoyl), Me ester:*
$C_{21}H_{35}NO_5$ 381.511
Isol. from *Fasciospongia cavernosa.*

N-*(2-Acetoxy-2-pentadecenoyl), Me ester:*
$C_{22}H_{37}NO_5$ 395.538
Isol. from *Fasciospongia cavernosa.*

N-*(15-Methyl-8-hexadecenoyl), Me ester:* ***Hurghamide E***
[330203-64-0]
$C_{22}H_{39}NO_3$ 365.555
Isol. from a *Hippospongia* sp. Wax.
λ_{max} 205 (ε 14700) (MeOH).

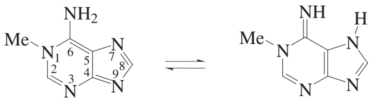
N-*(2-Alkylcyclopropyl)alkanoyl, Me ester (1):* ***Hurghamide F***
[330203-65-1]
$C_{22}H_{39}NO_3$ 365.555
Isol. from a *Hippospongia* sp. Wax. Posn. of cyclopropyl ring in side-chain not yet determined.

N-*(2-Alkylcyclopropylalkanoyl), Me ester (2):* ***Hurghamide G***
[330203-66-2]
$C_{24}H_{43}NO_3$ 393.609
Isol. from a *Hippospongia* sp. Wax. Posn. of cyclopropyl not determined.

Kashman, Y. *et al., Tetrahedron*, 1973, **29**, 3655 (*isol*)
Yunker, M.B. *et al., Tet. Lett.*, 1978, 4651 (*isol*)
Holm, A. *et al., Tet. Lett.*, 1980, 1125 (*synth*)
Neeman, J. *et al., Arch. Toxicol.*, Suppl., 1983, **6**, 258 (*isol*)
Jackson, W.R. *et al., Tet. Lett.*, 1988, **29**, 1983 (*synth*)
Isaac, B.G. *et al., J. Antibiot.*, 1991, **44**, 795 (*isol*)
Guo, Y. *et al., Nat. Prod. Lett.*, 1997, **9**, 281-288 (*Hurghamides A-D*)
Venkateswarlu, Y. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 832-834 (*N-2-acetoxy-2-alkenoyl derivs*)
Ramesh, P. *et al., Biochem. Syst. Ecol.*, 1999, **27**, 661-662 (*2-oxoalkyl derivs, isol, Sinularia*)
Guo, Y.-W. *et al., J. Asian Nat. Prod. Res.*, 2000, **2**, 251-256 (*Hurghamides E-G*)

6-Amino-1-methylpurine A-842

*1-Methyl-1*H*-purin-6-amine, 9CI. 1-Methyladenine. 1-Methyl-6-iminopurine.* ***Spongopurine***
[5142-22-3]



$C_6H_7N_5$ 149.155
Exists in the imino form in nonpolar solvs. and the amino form in H_2O. Isol. from starfishes *Asterias amurensis*, *Asterias rubens* and *Marthasterias glacialis*, and sponges *Geodia gigas* and *Hymeniacidon sanguinea*. Spawning-inducing factor in *Asterias*. Cryst. (H_2O). Mp 296-299° dec. pK_{a1} 7.2; pK_{a2} 11.

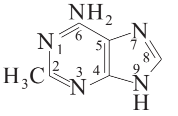
Picrate: Mp 255-257°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 714A (*ir*)
Ackermann, D. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1958, **312**, 210-213; 1961, **323**, 192-193 (*isol, ir, struct*)
Brookes, P. *et al., J.C.S.*, 1960, 539-545 (*synth*)

Karatani, H. *et al., Nature (London)*, 1969, **221**, 273-274 (*isol*)
Lichtenberg, D. *et al., J. Magn. Reson.*, 1972, **6**, 600-604 (*nmr*)
Garrett, E.R. *et al., J.A.C.S.*, 1972, **94**, 8532-8541 (*synth, uv*)
Doree, M. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1976, **73**, 1669-1673 (*biochem, bibl*)
Dreyfus, M. *et al., J.A.C.S.*, 1977, **99**, 7027-7037 (*tautom, bibl*)
Cimino, G. *et al., J. Nat. Prod.*, 1985, **48**, 523-528 (*isol, pmr*)

6-Amino-2-methylpurine A-843

*2-Methyl-1*H*-purin-6-amine, 9CI. 2-Methyladenine*
[1445-08-5]



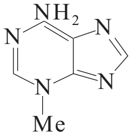
$C_6H_7N_5$ 149.155
Obt. by hydrol. of RNAs. Cryst. (EtOH). Mp 350°.

▶ AU6519000

Robins, R.K. *et al., J.A.C.S.*, 1953, **75**, 263 (*synth*)
Littlefield, J.W. *et al., Biochem. J.*, 1958, **70**, 642 (*isol*)
Starr, J.L. *et al., J. Biol. Chem.*, 1964, **239**, 3457 (*isol*)
Huynh-Dinh, T. *et al., J. Het. Chem.*, 1975, **12**, 111 (*synth, ir, pmr, uv, ms*)

6-Amino-3-methylpurine A-844

*3-Methyl-3*H*-purin-6-amine, 9CI. 3-Methyladenine, 8CI*
[5142-23-4]



$C_6H_7N_5$ 149.155
Isol. from the marine sponges *Plakortis* aff. *simplex* and *Topsentia genitrix*. Cryst. (H_2O). Mp 300° (291-292° dec.). pK_a 6.1. λ_{max} 273 (ϵ 14000) (MeOH) (Derep). λ_{max} 273 (ϵ 14010) (MeOH) (Berdy).

▶ AU6520000

9-β-D-Ribofuranosyl: 3-Methyladenosine
[72055-63-1]
$C_{11}H_{15}N_5O_4$ 281.271
Plates (MeOH) (as tosylate salt). Mp 150° dec. (tosylate salt). $[\alpha]_D^{20}$ -28.2 (c, 1.00 in H_2O) (tosylate salt). Imino at C-6.

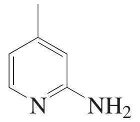
9-(2-Deoxy-β-D-ribofuranosyl): 2′-Deoxy-3-methyladenosine
[76227-26-4]
$C_{11}H_{15}N_5O_3$ 265.271
Powder (as tosylate salt). Mp 120° dec. (tosylate salt). Imino at C-6.

7-Oxide:
$C_6H_7N_5O$ 165.154
Sl. dark prisms. Mp 250-260° (dec.).

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 217A (*nmr*)
Brookes, P. *et al., J.C.S.*, 1960, 539 (*synth*)
Denayer, R. *et al., Bull. Soc. Chim. Fr.*, 1962, 1358 (*synth, uv*)
Jones, J.W. *et al., J.A.C.S.*, 1962, **84**, 1914 (*synth, uv*)
Elion, G.B. *et al., J.O.C.*, 1962, **27**, 2478 (*synth, uv*)
Pal, B.C. *et al., J.C.S.*, 1964, 400 (*ir, cryst struct*)
Lichtenberg, D. *et al., J. Magn. Reson.*, 1972, **6**, 600 (*nmr*)
Yamauchi, K. *et al., J.O.C.*, 1975, **40**, 385 (*synth*)
Stoller, C. *et al., J. Nat. Prod.*, 1988, **51**, 383 (*isol, uv, pmr, cmr, ms*)
Fujii, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2601 (*nucleosides*)
Itaya, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2025 (*7-oxide*)
Rudi, A. *et al., J. Nat. Prod.*, 2003, **66**, 682-685 (*isol, pmr, cmr*)

2-Amino-4-methylpyridine A-845

2-Amino-γ-picoline. 4-Methyl-2-pyridinamine, 9CI. W 45
[695-34-1]



$C_6H_8N_2$ 108.143
Alkaloid from *Acacia rigidula*. Analgesic, cardiac stimulant. Leaflets (petrol). Mp 98°. Bp 200-250°. pK_a 7.38. Sublimes. Component of Ascensil.

▶ LD_{50} (rat, orl) 200 mg/kg. TJ5150000

Hydrochloride: [2403-84-1]
Prisms (EtOH). Mp 176-177°.

Camphorsulfonate: Piricardio. Varunax
[12261-97-1]

N-*Ac:* [5327-32-2]
$C_8H_{10}N_2O$ 150.18
Prisms (C_6H_6). Mp 102-103° Mp 75-76°.

N-*Benzoyl:* [33120-20-6]
$C_{13}H_{12}N_2O$ 212.251
Cryst. (petrol). Mp 114°.

N-*Me:* [45699-12-5]
$C_7H_{10}N_2$ 122.169
Mp 90-92°.

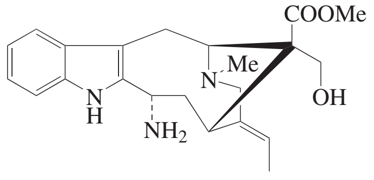
N-*Benzyl:* [13021-71-1]
$C_{13}H_{14}N_2$ 198.267
Cryst. (EtOH aq.). Mp 98-100°.

N-*Nitro:* [33245-30-6]
$C_6H_7N_3O_2$ 153.14
Solid. Mp 220°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 771B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 298C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1539B (*ir*)
Seide, O. *et al., Ber.*, 1924, **57**, 791-794 (*synth, derivs*)
Sprinzak, Y. *et al., J.A.C.S.*, 1956, **78**, 3207-3208 (*N-benzyl*)
Marchetti, G. *et al., Arch. Int. Pharmacodyn. Ther.*, 1963, **143**, 385-400 (*pharmacol*)
Clement, B.A. *et al., Phytochemistry*, 1998, **49**, 1377-1380 (*isol*)
Bhattacharya, A. *et al., Org. Process Res. Dev.*, 2007, **11**, 885-888 (*N-nitro*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ALC250

3-Amino-N^b-methylseco-voacarpine A-846

[169133-06-6]

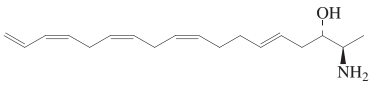


Absolute Configuration

$C_{22}H_{29}N_3O_3$ 383.489
Alkaloid from leaves of *Hunteria zeylanica* (Apocynaceae). Mp 154-155°.

Subhadhirasakul, S. *et al., Heterocycles*, 1995, **41**, 2049-2056 (*isol, uv, pmr, cmr, ms, cd, struct*)

2-Amino-5,9,12,15,17-octadecapentaen-3-ol, 9CI A-847



$C_{18}H_{29}NO$ 275.433

(2*R*,3*S*,5*E*,9*Z*,12*Z*,15*Z*)-*form*
Crucigasterin 275
[150151-84-1]
Isol. from *Pseudodistoma crucigaster*. Light yellow oil. λ_{max} 204 (ϵ 6200); 227 (ϵ 8700) (MeOH).

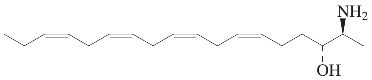
N,O-*Di-Ac:* [149849-81-0]
Oil. $[\alpha]_D^{29}$ +36 (c, 0.26 in MeOH).

17,18-Dihydro: 2-Amino-5,9,12,15-octadecatetraen-3-ol, 9CI. ***Crucigasterin 277***
[150151-83-0]
$C_{18}H_{31}NO$ 277.449
Isol. from *Pseudodistoma crucigaster*. Oil. λ_{max} 204 (ϵ 7900) (MeOH).

17,18-Dihydro, N,O-*di-Ac:* [149849-80-9]
Oil. $[\alpha]_D^{23}$ +36 (c, 0.53 in MeOH).

Jares-Erijman, E.A. *et al., J.O.C.*, 1993, **58**, 5732-5737 (*isol*)
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*abs config*)

2-Amino-6,9,12,15-octadeca-tetraen-3-ol A-848



$C_{18}H_{31}NO$ 277.449

(2*S*,3*R*,6*Z*,9*Z*,12*Z*,15*Z*)-*form*
Obscuraminol A. *Halaminol D*
[350484-80-9]
Isol. from the tunicate *Pseudodistoma obscurum*. Oil. $[\alpha]_D^{20}$ +5 (c, 0.14 in MeOH). $[\alpha]_D$ -23 (c, 0.78 in MeOH) (as di-Ac).

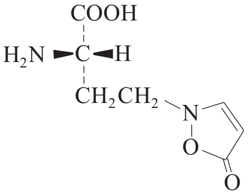
Clark, R.J. *et al., J. Nat. Prod.*, 2001, **64**, 1568-1571 (*Halaminol D*)

Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*Obscuraminol A*)

α-Amino-5-oxo-2(5*H*)-isoxazolebutanoic acid, 9CI A-849

α-Amino-γ-(isoxazolin-5-on-2-yl)butyric acid

[60102-46-7]



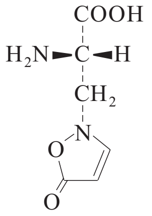
$C_7H_{10}N_2O_4$ 186.167

Isol. from sweet pea root exudates. Cryst. L-Config. not stated but presumed on biogenetic grounds.

Van Rompuy, L. *et al., J.C.S. Perkin 1*, 1973, 2503 (*pmr, uv*)
Lambein, F. *et al., Biochem. Biophys. Res. Commun.*, 1974, **61**, 155 (*isol, struct, uv, pmr*)
Kuo, Y.H. *et al., Arch. Int. Physiol. Biochim.*, 1976, **84**, 169 (*isol*)

α-Amino-5-oxo-2(5*H*)-isoxazolepropanoic acid, 9CI A-850

α-Amino-5-oxo-3-oxazoline-2-propionic acid, 8CI. β-(Isoxazolin-5-on-2-yl)alanine. 2-Alanyl-3-isoxazolin-5-one



$C_6H_8N_2O_4$ 172.14

***(S)*-form**

L-form

[59476-61-8]

Amino acid from the roots of pea seedlings (*Pisum* spp.) and *Lathyrus* spp. Fairly sol. H_2O. Mp 203-205° dec. $[\alpha]_D^{20}$ -62 (c, 1.4 in H_2O). Base-labile. λ_{max} 265 (ε 12300) (pH 2 buffer) (Berdy). λ_{max} 267 (ε 13190) (pH 10 buffer) (Berdy).

N-*(4-Amino-4-carboxybutanoyl): γ-Glutamyl-β-(isoxazolin-5-on-2-yl)alanine*
[142115-24-0]
$C_{11}H_{15}N_3O_7$ 301.255
Constit. of *Lens culinaris* (lentil) and some *Lathyrus* spp. Cryst. (Me_2CO aq.).

Lambein, F. *et al., Biochem. Biophys. Res. Commun.*, 1969, **37**, 375 (*isol*)
Lambein, F. *et al., Heterocycles*, 1976, **4**, 567 (*isol*)
Baldwin, J.E. *et al., Tet. Lett.*, 1985, **26**, 5931 (*synth, pmr, ir*)
Lambein, F. *et al., Phytochemistry*, 1992, **31**, 887 (*glutamyl deriv*)
Kuo, Y.-H *et al., Phytochemistry*, 1998, **49**, 43-48 (*occur, metab, biosynth*)

8-Amino-7-oxononanoic acid, 9CI A-851

[4707-58-8]

$H_3CCH(NH_2)CO(CH_2)_5COOH$

$C_9H_{17}NO_3$ 187.238

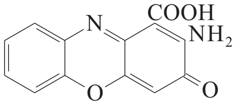
Isol. from *Penicillium chrysogenum* as a biotin intermediate. Cryst. (EtOH/Et_2O). Mp 133-134°.

Suyama, T. *et al., CA*, 1964, **60**, 4013 (*synth*)
Iwahara, S. *et al., Agric. Biol. Chem.*, 1966, **30**, 304
Eisenburg, M.A. *et al., Biochemistry*, 1970, **9**, 108

2-Amino-3-oxo-3*H*-phenoxazine-1-carboxylic acid A-852

*2-Amino-1-carboxy-3*H*-phenoxazin-3-one*

[14994-68-4]



$C_{13}H_8N_2O_4$ 256.217

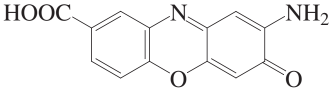
Prod. by a *Nocardia* strain. Dark orange needles. Sol. bases, MeOH, $CHCl_3$; poorly sol. H_2O, acids. Mp 310-320°. λ_{max} 233 (ε 28220); 425 (ε 10620); 442 (ε 10380) (EtOH) (Berdy). λ_{max} 230 ; 441 (HCl) (Berdy).

Gerber, N.N. *et al., Biochemistry*, 1966, **5**, 3824 (*isol, synth, uv, ir*)
Gerber, N.N. *et al., Can. J. Chem.*, 1968, **46**, 790 (*synth, ir*)

2-Amino-3-oxo-3*H*-phenoxazine-8-carboxylic acid A-853

***Umycin C**. SM 76. Antibiotic SM 76*

[149837-40-1]



$C_{13}H_8N_2O_4$ 256.217

Prod. by *Streptomyces* sp. DSM 3813. Anthelmintic. Red powder. λ_{max} 247 (ε 21900); 257 (ε 23400); 426 (ε 15800); 436 (ε 16200); 485 (sh) (ε 5010) (MeOH) (Derep).

N^2-*Ac: **Umycin A**. SM 35. Antibiotic SM 35*
[116511-07-0]
$C_{15}H_{10}N_2O_5$ 298.254
Prod. by *Streptomyces* sp. DSM 3813. Anthelmintic. Red powder.

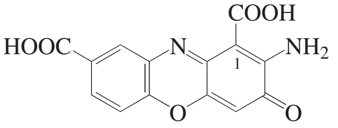
N^2-*Me: 2-(Methylamino)-3-oxo-3*H*-phenoxazine-8-carboxylic acid. **Texazone***
[87081-53-6]
$C_{14}H_{10}N_2O_4$ 270.244
Prod. by an *Actinomyces* strain WRAT-210. Dark red needles (Me_2CO). Sol. DMSO, Py; fairly sol. EtOAc, EtOH, Et_2O, $CHCl_3$; poorly sol. H_2O. Dec. without melting at 240°. λ_{max} 247 (ε 21900); 257 (ε 23400); 426 (ε 15800); 436 (ε 16200); 485 (sh) (ε 5010) (MeOH). λ_{max} 247 (ε 22000); 257 (ε 23440); 426 (ε 15850); 436 (ε 16218); 480 (ε 5110) (MeOH) (Berdy).

N^2-*Me, Et ester:* [87081-50-3]
Reddish-orange. Mp 256-257°.

N^2-*Me, amide: **Antibiotic BE 39907B**. BE 39907B*
[181469-60-3]
$C_{14}H_{11}N_3O_3$ 269.259
Prod. by *Saccharopolyspora* sp. A39907. Cytotoxic agent.

Gerber, N.N. *et al., J. Antibiot.*, 1983, **36**, 688 (*Texazone*)
Eur. Pat., 1988, 260 486; *CA*, **109**, 142586p (*Umycins*)
Japan. Pat., 1996, 96 198 861; *CA*, **125**, 219739f (*BE 39907B*)

2-Amino-3-oxo-3*H*-phenoxazine-1,8-dicarboxylic acid A-854



$C_{14}H_8N_2O_6$ 300.227

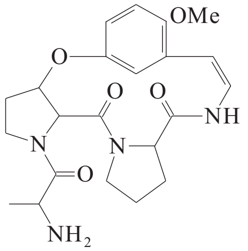
*1-Amide: 8-Amino-9-(aminocarbonyl)-7-oxo-7*H*-phenoxazine-2-carboxylic acid. **Elloxazinone B***
[943756-13-6]
$C_{14}H_9N_3O_5$ 299.242
Prod. by *Streptomyces griseus* Acta 2871. Antitumour agent. Red solid. λ_{max} 240 (log ε 2.12); 256 (log ε 1.93); 412 (log ε 1.42); 431 (log ε 1.5) (MeOH).

*1-Amide, 8-Me ester: **Elloxazinone A***
[943756-12-5]
$C_{15}H_{11}N_3O_5$ 313.269
Prod. by *Streptomyces griseus* Acta 2871. Red solid. λ_{max} 239 (log ε 2.73); 259 (log ε 2.57); 411 (log ε 2.07); 428 (log ε 2.09) (MeOH).

Graf, E. *et al., J. Antibiot.*, 2007, **60**, 277-284 (*isol, uv, pmr, cmr, activity*)

1-(2-Amino-1-oxopropyl)-2,3,3*a*,13*a*,14,15,16,18*a*-octahydro-8-methoxy-5,9-metheno-9*H*-dipyrrolo[3,2-*b*:1′,2′-*e*][1,5,8]oxadiazacyclopentadecine-13,18(1*H*,12*H*)-dione, 9CI A-855

[147471-65-6]

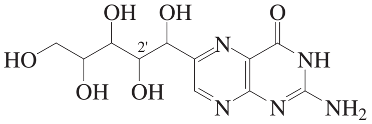


$C_{22}H_{28}N_4O_5$ 428.487

Related to the Zizyphines. Alkaloid from flowers of *Sphaeranthus indicus* (Asteraceae). Mp 72°.

Chughtai, M.I.D. *et al., Sci. Int. (Lahore)*, 1992, **4**, 151; *CA*, **118**, 230141f (*isol, struct*)

2-Amino-6-(1,2,3,4,5-pentahydroxypentyl)-4(1*H*)-pteridinone A-856



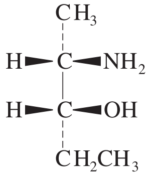
$C_{11}H_{15}N_5O_6$ 313.269
Cryst. (EtOH aq.). $[\alpha]_D$ +3.7 (c, 0.1 in NH_4OH aq.).

2′-O-β-D-Glucuronopyranoside:
$C_{17}H_{23}N_5O_{12}$ 489.395
Isol. from cultures of *Mycobacterium phlei* and *Mycobacterium smegmatis.* Mp 250-280° (dec.). $[\alpha]_D^{25}$ +7.2 (c, 0.26 in H_2O).

Goto, M. *et al., Annalen*, 1965, **689**, 221 (*isol, uv, ir, ms*)

2-Amino-3-pentanol, 9CI A-857

[116836-16-9]



(2*S*,3*R*)-*form*

$C_5H_{13}NO$ 103.164

(2*S*,3*R*)-*form* [111061-02-0]
Oil. $[\alpha]_D^{23}$ +14 (c, 1 in $CHCl_3$).

N-*Ac:* [138145-16-1]
$C_7H_{15}NO_2$ 145.201
Isol. from the fungus *Scolecotrichum graminis.* $[\alpha]_D^{22}$ -25 (c, 1 in EtOH).

N,N-*Dibenzyl:* [111060-70-9]
$C_{19}H_{25}NO$ 283.413
Oil. $[\alpha]_D^{23}$ +48.2 (c, 1 in $CHCl_3$).

(2*S*,3*S*)-*form* [180187-00-2]
Solid (hexane). Mp 67-68°. $[\alpha]_D^{23}$ -15.9 (c, 0.34 in MeOH).

N-*Ac:* [138145-17-2]
Isol. from *Scolecotrichum graminis.* $[\alpha]_D^{22}$ -188 (c, 0.5 in EtOH).

N,N-*Dibenzyl:* [111060-69-6]
Oil. $[\alpha]_D^{23}$ +70.5 (c, 1 in $CHCl_3$).

(2*RS*,3*RS*)-*form*
(±)-threo-*form*
[147975-87-9]
Mp 104-105° (as oxalate).

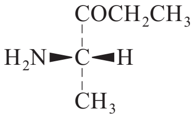
(2*RS*,3*SR*)-*form*
(±)-erythro-*form*
[147975-86-8]
Mp 124-126° (as oxalate).

[141824-38-6 , 599207-02-0]

Reetz, M.T. *et al., Angew. Chem., Int. Ed.*, 1987, **26**, 1141-1143 (*synth*)
Tabuchi, H. *et al., Agric. Biol. Chem.*, 1991, **55**, 2669-2671 (*N-Ac, isol*)
Andrés, J.M. *et al., J.O.C.*, 1996, **61**, 4210-4213 (*synth, ir, pmr, cmr*)

Ueda, S. *et al., Bioorg. Med. Chem.*, 2004, **12**, 4101-4116 (*synth, pmr*)

2-Amino-3-pentanone A-858



$C_5H_{11}NO$ 101.148

(*S*)-*form* [138145-15-0]

N-*Ac:* ***2-Acetamido-3-pentanone***
$C_7H_{13}NO_2$ 143.185
Isol. from the fungus *Scolecotrichum graminis.* $[\alpha]_D^{25}$ -69.8 (c, 1 in EtOH).

(±)-*form* [93222-93-6]
Off-white cryst. (as hydrochloride). Mp 127-129° (hydrochloride). CAS no. refers to hydrochloride.

N,N-*Di-Me:* [71504-23-9]
$C_7H_{15}NO$ 129.202
Bp_{40} 63-64°.

[79851-68-6]

Coffen, D.L. *et al., J.O.C.*, 1984, **49**, 5109 (*synth*)
Tabuchi, H. *et al., Agric. Biol. Chem.*, 1991, **55**, 2669 (*isol, deriv, synth*)
Collina, S. *et al., Tetrahedron: Asymmetry*, **10**, 2387-2397 (*N,N-di-Me, synth*)

(5-Aminopentyl)guanidine, 9CI A-859

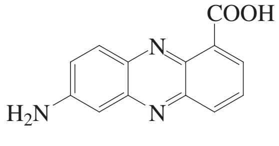
1-Amino-5-guanidinopentane. ***Homoagmatine***
[18431-52-2]
$HN{=}C(NH_2)NH(CH_2)_4CH_2NH_2$
$C_6H_{16}N_4$ 144.219
Constit. of *Lathyrus sativus* (chickling pea). Major intermed. in homoarginine metab. pathway. Mp 135-137° (as hydrochloride).

N^5-*Ac:* ***Acetylhomoagmatine***
[180251-16-5]
$C_8H_{18}N_4O$ 186.256
Constit. of *Cliona celata.* Yellow amorph. solid. λ_{max} 206 (log ϵ 3.23) (MeOH).

Ramakrishna, S. *et al., Phytochemistry*, 1973, **12**, 2691-2695 (*isol, synth, ir*)
Lenis, L.A. *et al., Nat. Prod. Lett.*, 1996, **8**, 15-23 (*Acetylhomoagmatine*)
Castellanos, L. *et al., Mar. Drugs*, 2006, **4**, 286-289 (*Acetylhomoagmatine, synth*)

7-Amino-1-phenazinecarboxylic acid, 8CI A-860

[24827-33-6]



$C_{13}H_9N_3O_2$ 239.233
Red needles ($PhNO_2$). Mp 340° dec.

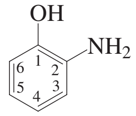
Me ester: [24535-36-2]
$C_{14}H_{11}N_3O_2$ 253.26
Red needles (toluene). Mp 202-204°.

N^5-*Me, betaine: 7-Amino-1-carboxy-5-methylphenazinium hydroxide inner salt, 9CI.* ***Aeruginosin A****. Eruginosin A*
[21668-67-7]
$C_{14}H_{11}N_3O_2$ 253.26
Pigment from *Pseudomonas aeruginosa.* Insol. nonpolar. solvs., sol. H_2O, acids, bases, poorly sol. butanol, hexane. Red-purple fluor. in uv light. Dec. on heating. λ_{max} 235 (ϵ 31620); 280 (ϵ 44670); 396 (ϵ 11750); 515 (ϵ 14120) (pH 7 buffer) (Berdy). λ_{max} 235 ; 285 ; 380 ; 538 (HCl) (Berdy). λ_{max} 235 ; 275 ; 375 ; 525 (NaOH aq.) (Berdy).

Holliman, F.G. *et al., Tetrahedron*, 1963, **19**, 1841-1848 (*synth, Me ester*)
Hansford, G.S. *et al., J.C.S. Perkin 1*, 1972, 103 (*betaine, synth, biosynth*)

2-Aminophenol, 9CI A-861

o-*Hydroxyaniline. 1-Amino-2-hydroxybenzene.* ***Questiomycin B***
[95-55-6]
[27598-85-2]



C_6H_7NO 109.127
Manuf. by redn. of 2-nitrophenol. Isol. from *Streptomyces* sp. and *Penicillium notatum.* Also isol. from a purple bacterium from a sponge of *Adocia* sp. Electrochem. polym. gives electroactive polymer films. Dye intermediate. Tuberculostatic. Possesses antibacterial props. Cryst. (H_2O). Sol. MeOH, H_2O, Et_2O, EtOAc; fairly sol. CCl_4; poorly sol. hexane. Mp 174°. pK_{a1} 4.78; pK_{a2} 9.97 (20°). Free base readily oxidised. λ_{max} 235 (ϵ 28400); 467 (ϵ 1700) (0.25*N* HCl) (Derep). λ_{max} 335 (ϵ 1230) (0.1*N* KOH) (Derep). λ_{max} 240 (ϵ 26300); 435 (ϵ 2330) (pH 7.4) (Derep). λ_{max} 229 ; 283 (H_2O) (Berdy). λ_{max} 268 (HCl) (Berdy). λ_{max} 300 (NaOH) (Berdy).

▶ Eye and respiratory tract irritant. LD_{50} (rat, orl) 1300 mg/kg. LD_{50} (mus, ipr) 350 mg/kg. Exp. reprod. and teratogenic effect. SJ4950000

Hydrochloride: [51-19-4]
Mp 207°.

▶ SJ6069000

N-*Formyl:* N-*(2-Hydroxyphenyl)formamide, 9CI. 2-Hydroxyformanilide.* N-*Formylquestiomycin B*
[2843-27-8]
$C_7H_7NO_2$ 137.138
Prod. by *Penicillium notatum.* Needles (H_2O). Mp 129-129.5°. λ_{max} 218 (ϵ 10280); 245 (ϵ 11910); 286 (ϵ 6295) (MeOH) (Berdy).

N-*Ac: 2-Acetamidophenol. 2-Hydroxyacetanilide.* N-*(2-Hydroxyphenyl)acetamide*
[614-80-2]
$C_8H_9NO_2$ 151.165

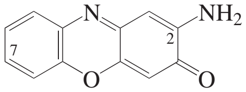
Prod. by *Streptomyces* sp. Plates (EtOH). Sol. hot H_2O. Mp 209°.

▶ Eye irritant. AE4025000

Anzai, K. *et al., J. Antibiot., Ser. A*, 1960, **13**, 125 (*isol*)
Pfeifer, S. *et al., Pharmazie*, 1972, **27**, 536-542 (*isol*)
Oclarit, J.M. *et al., Fish. Sci.*, 1994, **60**, 559 (*isol*)
Pusecker, K. *et al., J. Antibiot.*, 1997, **50**, 479 (*N-Ac, isol, ir, pmr, ms*)
Rahaim, R.J. *et al., Synthesis*, 2006, 3316-3340 (*synth, pmr, cmr, N-Ac*)

2-Amino-3*H*-phenoxazin-3-one, 9CI, 8CI **A-862**

Questiomycin A. *AV toxin C*
[1916-59-2]



$C_{12}H_8N_2O_2$ 212.207
Isol. from *Acrospermum viticola, Brevibacterium iodinum, Calocybe gambosa* (St George's mushroom), *Microbispora aerata, Streptomyces thioluteus, Pycnoporus* sp., *Waksmania* sp., and mushroom *Lepiota americana*. Used as a 1m*M* soln. in EtOH as redox indicator for titanometric detn. of Fe(*III*), Au(*III*), $Cr_2O_7^{2\ominus}$, $VO_4^{3\ominus}$ and some organic compds.; redox indicator for stannometry. Aromatase and sulfatase inhibitor. Active against gram-positive bacteria, mycobacteria, *Candida albicans* and shows antitumour activity. Phytotoxin. Dark brown or red cryst. (EtOH). Sol. EtOH. Subl. 255-257. Sometimes occurs in amorph. form with Mp 296-297°. E° + 0.372V (pH 0.92, 23°). λ_{max} 235 (ϵ 28400); 467 (ϵ 1700) (0.25*N* HCl) (Derep). λ_{max} 335 (ϵ 1230) (0.1*N* KOH) (Derep). λ_{max} 240 (ϵ 26300); 435 (ϵ 2330) (pH 7.4) (Derep).

▶ LD_{50} (mus, ipr) 200 mg/kg. SP7695000

*N-β-*D*-Glucopyranosyl:* **N-*β*-D-*Glucopyranosylquestiomycin A***
$C_{18}H_{18}N_2O_7$ 374.349
Prod. by *Microbispora* sp. TP-A0184. Antibacterial and cytotoxic agent. Red powder. Sol. DMSO, Py; fairly sol. MeOH; poorly sol. $CHCl_3$, EtOAc. Mp > 195° dec. $[\alpha]_D^{28}$ +16.5 (c, 0.1 in Py). λ_{max} 240 (log ϵ 4.33); 423 (log ϵ 4.23) (MeOH).

N-*Ac:* N-*(3-Oxo-3*H*-phenoxazin-2-yl)acetamide, 9CI. 2-Acetamido-3*H*-phenoxazin-3-one.* **N-*Acetylquestiomycin A***
[1916-55-8]
$C_{14}H_{10}N_2O_3$ 254.245
From *Brevibacterium iodinum*, *Microbispora aerata*, *Streptomyces thioluteus* and *Waksmania aerata*. Used as a 1m*M* soln. in EtOH as redox indicator for titanometric detn. of Fe(*III*), Au(*III*), Ce(*IV*), $Cr_2O_7^{2\ominus}$, $VO_4^{3\ominus}$ and some organic compounds. Active against *Sarcina lutea* and *Trichophyton* sp. Orange cryst. Sol. EtOH, Et_2O, C_6H_6, MeOH; poorly sol. H_2O. Subl. 165°. E° + 0.375V (pH 0.84, 23°). λ_{max} 240 (E1%/1cm 1400); 405 (E1%/1cm 1100) (EtOH) (Berdy).

N-*Hydroxyacetyl:* N-*Hydroxyacetylquestiomycin A*. ***Chandrananimycin B***
$C_{14}H_{10}N_2O_4$ 270.244
Prod. by a marine *Actinomadura* sp. M045. Orange solid. λ_{max} 238 (log ϵ 3.85); 399 (log ϵ 3.66) (MeOH).

*6-Hydroxy: 2-Amino-6-hydroxy-3*H*-phenoxazin-3-one.* ***6-Hydroxyquestiomycin A***
$C_{12}H_8N_2O_3$ 228.207
Prod. by the marine *Halomonas* sp. GWS-BW-H8hM. Red solid. λ_{max} 236 (log ϵ 3.93); 277 (log ϵ 3.75); 430 (log ϵ 3.72) (MeOH). λ_{max} 230 (log ϵ 3.91); 284 (log ϵ 3.61); 464 (log ϵ 3.5) (MeOH/HCl).

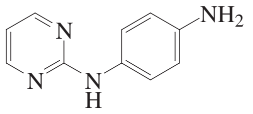
9-Hydroxy, N-*Ac:* N-*Acetyl-9-hydroxyquestiomycin A*. ***Chandrananimycin A***
$C_{14}H_{10}N_2O_4$ 270.244
Prod. by a marine *Actinomadura* sp. M048. Orange solid. λ_{max} 226 (log ϵ 4.52); 270 (log ϵ 4.38); 423 (log ϵ 4.45) (MeOH).

*7,8-Dimethoxy: 2-Amino-7,8-dimethoxy-3*H*-phenoxazin-3-one. 7,8-Dimethoxyquestiomycin A*. ***Peristrophine***
$C_{14}H_{12}N_2O_4$ 272.26
Alkaloid from *Peristrophe roxburghiana*. Mp 250° dec. λ_{max} 235 ; 280 (sh) ; 484 (MeOH). λ_{max} 239 ; 273 (sh) ; 320 (sh) ; 544 (sh) ; 583 (MeOH/HCl).

Fischer, O. *et al., Ber.*, 1961, **27**, 2784 (*synth*)
Gerber, N.N. *et al., Biochemistry*, 1964, **3**, 598; 1966, **5**, 3824 (*isol, uv, ir*)
Gerber, N.N. *et al., J.O.C.*, 1967, **32**, 4055 (*isol, uv, ir, bibl*)
Ruzička, E. *et al., Mikrochim. Acta*, 1967, 277 (*use*)
Ruzička, E. *et al., CA*, 1968, **69**, 40930j (*stannometry*)
Ikekawa, T. *et al., Chem. Pharm. Bull.*, 1968, **16**, 1705 (*synth, ir*)
Sullivan, G. *et al., J. Pharm. Sci.*, 1971, **60**, 1097 (*isol*)
Baer, H. *et al., Pharmazie*, 1971, **26**, 108; 314 (*isol*)
Hishida, T. *et al., Chem. Lett.*, 1974, 293 (*synth*)
Schlunegger, U.V. *et al., Helv. Chim. Acta*, 1976, **59**, 1383 (*isol*)
Motohashi, N. *et al., Yakugaku Zasshi*, 1983, **103**, 364 (*synth, props*)
Bolognese, A. *et al., J. Het. Chem.*, 1986, **23**, 1003 (*synth, pmr, uv, deriv*)
Kinjo, J. *et al., Tet. Lett.*, 1987, **28**, 3697 (*isol*)
Simandi, L.I. *et al., Tet. Lett.*, 1993, **34**, 717 (*synth*)
Igarashi, Y. *et al., J. Antibiot.*, 1998, **51**, 915-920 (*Glucosylquestiomycin A*)
Qin, J.P. *et al., Yaoxue Xuebao*, 1999, **34**, 599-603 (*Peristrophine*)
Kim, D.S. *et al., Planta Med.*, 2000, **66**, 78 (*Questiomycin A, isol, activity*)
Bolognese, A. *et al., J. Med. Chem.*, 2002, **45**, 5205-5216 (*synth, N-Ac, uv, pmr*)
Maskey, R.P. *et al., J. Antibiot.*, 2003, **56**, 622-629 (*Chandrananimycins*)
Bitzer, J. *et al., J. Antibiot.*, 2006, **59**, 86-92 (*6-Hydroxyquestiomycin A*)
Giurg, M. *et al., Pol. J. Chem. (Rocz. Chem.)*, 2006, **80**, 297-306 (*synth*)
Giurg, M. *et al., Synth. Commun.*, 2007, **37**, 1779-1789 (*synth, ir, uv, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, QCJ275

2-[(4-Aminophenyl)amino]pyrimidine **A-863**

N-*(2-Pyrimidinyl)-1,4-benzenediamine*
[743449-54-9]

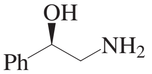


$C_{10}H_{10}N_4$ 186.216
Alkaloid from the bulbs of *Scilla maderensis.* α_1-Adrenoceptor antagonist. Needles (MeOH). Mp 270-271°. λ_{max} 213 ; 270 (MeOH).

Dias, C. *et al., Planta Med.*, 2003, **69**, 1060-1062 (*isol, pmr, cmr, ms*)

2-Amino-1-phenylethanol **A-864**

α-Aminomethylbenzenemethanol, 9CI. α-(Aminomethyl)benzyl alcohol, 8CI. β-Amino-α-hydroxyethylbenzene. (Aminomethyl)phenylcarbinol. 2-Hydroxy-2-phenylethylamine. 1-Phenylethanolamine. ***Resedinine***†. *Apophedrin. Norphedrin. Bisnorephedrine*
[7568-93-6]



(*R*)*-form*

$C_8H_{11}NO$ 137.181
Log P 0.27 (calc).

▶ LD_{50} (mus, ipr) 250 mg/kg. DN5500000

(*R*)*-form* [2549-14-6]
Mp 54-58°. $[\alpha]_D^{20}$ -42.2 (c, 1 in EtOH).

O-*Benzoyl:* [111025-00-4]
$C_{15}H_{15}NO_2$ 241.289
Isol. from *Oxytropis pseudoglandulosa*. Needles (pentane). Mp 38-40°. $[\alpha]_D^{21}$ +181.9 (c, 2.275 in MeOH).

N-*Benzoyl:* N-*Benzoyl-2-hydroxy-2-phenylethylamine. 2-(Benzoylamino)-1-phenylethanol*
[111059-46-2]
$C_{15}H_{15}NO_2$ 241.289
Constit. of *Oxytropis pseudoglandulosa* (Fabaceae). Plates (MeOH/Et_2O). Mp 151-152° (143-144°). $[\alpha]_D^{24}$ -16.2 (c, 0.81 in MeOH). $[\alpha]_D$ -21 (c, 0.7 in MeOH).

N-*(3-Pyridinecarbonyl):* **N-*Nicotinoyl-2-hydroxy-2-phenylethylamine***. *2-(Nicotinoylamino)-1-phenylethanol*
[168780-03-8]
$C_{14}H_{14}N_2O_2$ 242.277
Isol. from aerial parts of *Oxytropis puberula*. Mp 157-158°. $[\alpha]_D$ -25.3 (c, 0.79 in MeOH).

N-*Me: Halostachine. α-[(Methylamino)methyl]benzenemethanol, 9CI. α-[(Methylamino)methyl]benzyl alcohol, 8CI. 2-(Methylamino)-1-phenethanol. β-Hydroxy-*N*-methylphenethylamine*
[495-42-1]
Alkaloid from *Halostachys caspica* (Chenopodiaceae). Hypertensive agent showing ephedrine-like activity. Mp 43-45°. $[\alpha]_D$ -47.

N-*Me, hydrochloride:* Mp 113-114°. $[\alpha]_D$ -52.4.

N,N-*Di-Me: 2-Dimethylamino-1-phenylethanol. α-[(Dimethylamino)methyl]benzenemethanol, 9CI. α-[(Dimethylamino)methyl]benzyl alcohol, 8CI.* N,N-*Dimethyl-1-phenylethanolamine.* ***Ubine***
[34469-09-5]
Alkaloid from *Dolichothele uberiformis* (Cactaceae), also detected by ms in *Dolichothele longimamma*. $Bp_{0.15}$ 58-60°. $[\alpha]_D^{25}$ -62.5 (c, 1.0 in MeOH). n_D^{25} 1.5164.

Me ether: 2-Methoxy-2-phenylethylamine. β-Methoxybenzeneethanamine, 9CI
[55163-76-3]
$C_9H_{13}NO$ 151.208
d_4^{20} 1.02. Bp_{20} 110-113°. $[\alpha]_D^{22}$ -118.5 (neat).

Me ether; hydrochloride: [62064-68-0]
Mp 158-159°.

▶SH8090000

(*S*)-*form* [56613-81-1]
Mp 61-62° (55-57°). $[\alpha]_D$ +47.9 (c, 2.4 in EtOH).

Hydrochloride: [71025-82-6]
Mp 209-210°. $[\alpha]_D^{13}$ +48.8 (c, 5.08 in H_2O).

N-*Ac:* [155073-71-5]
$C_{10}H_{13}NO_2$ 179.218
$[\alpha]_D$ +73 (c, 0.2 in $CHCl_3$) (>90% ee; room temp.).

N-*Benzoyl:* Constit. of *Oxytropis trichophysa* and *Oxytropis muricata*. Cryst. (Me_2CO). Mp 154-155°. $[\alpha]_D^{30}$ +35.2 (c, 0.68 in MeOH).

N-*Benzoyl,* O-*Ac: 2-Acetyloxy-*N-*benzoyl-2-phenylethylamine.* ***Muricatide***
[111025-01-5]
[128820-22-4 , 109393-37-5]
$C_{17}H_{17}NO_3$ 283.326
Alkaloid from *Oxytropis muricata*. Needles (hexane/petrol). Mp 114-115° (110-112°). $[\alpha]_D^{20}$ +40.7 (c, 0.43 in $CHCl_3$). λ_{max} 208 (sh) ; 226 (EtOH).

N-tert-*Butyloxycarbonyl:*
$C_{13}H_{19}NO_3$ 237.298
Solid. Mp 66-68°. $[\alpha]_D^{20}$ +3.5 (c, 1 in EtOH) (99% ee).

N-*Me: 2-(Methylamino)-1-phenylethanol*
[65058-52-8]
$C_9H_{13}NO$ 151.208
Solid. Mp 45-47° (39-40°). $Bp_{0.1}$ 99-102°. $[\alpha]_D^{20}$ +40.41 (c, 1.89 in EtOH).

N,N-*Di-Me:* [2202-69-9]
[939-45-7]
Mp 113.5° (as hydrochloride). $[\alpha]_D^{23}$ +77.6 (c, 0.1 in EtOH).

N-*Benzyl:*
$C_{15}H_{17}NO$ 227.305
Cryst. (EtOAc/petrol). Mp 105-107°. $[\alpha]_D^{20}$ +33.8 (c, 2 in EtOH) (99% ee).

(±)-*form* [1936-63-6]
Pale yellow cryst. Mp 56-57°. Bp_{17} 160°. pK_{a1} 8.79; pK_{a2} 11.9 (25°, 0.1*M* KCl).

▶DA4727250

Sulfate: [50835-37-5]
Cryst. Mp 275-276°.

▶DA4729900

N-*Ac:* [3306-05-6]
$C_{10}H_{13}NO_2$ 179.218
Solid. Mp 125-126°.

N-*Benzoyl:* [96328-15-3]
Leaflets (EtOH). Mp 148-149.5°.

N-tert-*Butyloxycarbonyl:*
Solid. Mp 120-121°.

N-*Me:* [68579-60-2]
Cryst. (CH_2Cl_2/hexane). Mp 72-73°.

▶DA4976000

N,N-*Di-Me:* [2202-68-8]
[1797-76-8]
Isol. from leaves of *Aptenia cordifolia*, as partial racemate of low opt. rotn. Mp 144-145° (as hydrochloride)(synthetic). $[\alpha]_D^{25}$ +1.1 (c, 0.08 in $CHCl_3$) (nat.).

N-*Benzyl:*
Solid (EtOAc/petrol). Mp 93-96°.

Me ether: [3490-79-7]
Bp_{12} 103-105°.

(ξ)-*form*
Alkaloid from *Reseda luteola* (Resedaceae), also obt. by hydrol. of 5-Phenyl-2-oxazolidinone, P-347. Vasoconstrictor. Mp 112-114°. Prob. artifact. The identification is dubious in view of the Mp which is higher than that of either the chiral or racemic form of authentic substance.

O-*Benzoyl:* ***Trichophydine***. *Trichophidine*
[67031-54-3]
$C_{15}H_{15}NO_2$ 241.289
Isol. from epigeal parts of *Oxytropis trichophysa*. Cryst. (hexane/petrol). Mp 200-203° (as hydrochloride). It is claimed that a previous alkaloid, Mp 38-40°, isolated from *Oxytropis pseudoglandulosa* given this struct. was erroneous and that it is an oxazoline of undetermined struct.

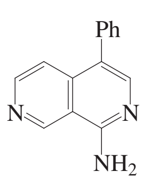
N,O-*Dibenzoyl:* ***Trichophysine***
$C_{22}H_{19}NO_3$ 345.397
Isol. from epigeal parts of *Oxytropis trichophysa*. Cryst. (hexane/Et_2O). Mp 100-103°.

[36297-03-7 , 61217-79-6 , 6027-95-8 , 6589-55-5 , 6853-14-1 (*N*-Me), 18867-43-1 , 80997-83-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1272B (*ir*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1277A (*N-Me, ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 585B (*N-Me, nmr*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 575C (*nmr*)
Rosenmund, K.W. *et al., Ber.*, 1913, **46**, 1034-1050 (*Me ether*)
Mannich, C. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1927, **2**, 10 (*Me ether*)
Men'shikov, G.P. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1943, **13**, 801; 1947, **17**, 1569; *CA*, **39**, 1172; **42**, 2245 (*N-Me, isol, struct, synth*)
Rebstock, M.C. *et al., J.A.C.S.*, 1951, **73**, 3666-3670 (*synth*)
Dornow, A. *et al., Chem. Ber.*, 1955, **88**, 1267-1275 (*synth*)
Schöpf, C. *et al., Annalen*, 1959, **626**, 150-154 (*abs config*)
Poos, G.I. *et al., J. Med. Chem.*, 1963, **6**, 266-272 (*synth*)
Lukes, R. *et al., CA*, 1964, **61**, 693g (*N-Me, abs config, synth*)
Reisch, J. *et al., Fresenius' Z. Anal. Chem.*, 1968, **238**, 29-35 (*nmr, struct*)
Cocolas, G.H. *et al., J. Pharm. Sci.*, 1971, **60**, 1749 (*N-di-Me, synth*)
Sabelli, H.C. *et al., Adv. Behav. Biol.*, 1974, **10**, 331 (*rev, props*)
Kirmse, W. *et al., Chem. Ber.*, 1975, **108**, 79-87 (*Me ether*)
Tadzhibaev, M.M. *et al., Khim. Prir. Soedin.*, 1976, **12**, 270-271; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 245-246 (*isol*)
Angeloni, A.S. *et al., Gazz. Chim. Ital.*, 1977, **107**, 421 (*N-di-Me, abs config*)
Ranieri, R.L. *et al., J. Nat. Prod.*, 1977, **40**, 173 (*N-di-Me, isol*)
Kruger, T.L. *et al., J.O.C.*, 1977, **42**, 4161 (*N-di-Me, ms, occur*)
Frank, H. *et al., Angew. Chem.*, 1978, **90**, 396-398 (*glc, resoln*)
Kniezo, L. *et al., Coll. Czech. Chem. Comm.*, 1978, **43**, 1917-1923 (*synth*)
Wehrli, H. *et al., Helv. Chim. Acta*, 1980, **63**, 1915 (*N-Me, synth, ir, pmr*)
Meyers, A.I. *et al., J.O.C.*, 1980, **45**, 2785-2791 (*synth*)
Shannon, H.E. *et al., J. Pharmacol. Exp. Ther.*, 1981, **217**, 379-385 (*pharmacol, rev*)
Midland, M.M. *et al., J.O.C.*, 1985, **50**, 3237-3239 (*synth*)
Coote, S.J. *et al., J.C.S. Perkin 1*, 1989, 2223-2228 (*S-form, N-Me, synth, ir, pmr, cmr*)
Ziegler, T. *et al., Synthesis*, 1990, 575-578 (*R-form, synth, pmr*)
Brussee, J. *et al., Tetrahedron*, 1990, **46**, 1653-1658 (*R-form, synth*)
Izumi, T. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 1216-1221 (*Muricatide, synth*)
Akhmedzhanova, V.I. *et al., Khim. Prir. Soedin.*, 1993, **29**, 90-91; 1994, **30**, 414-416; 1996, **32**, 212-216; 1997, **33**, 424-427; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 76; 1994, **30**, 379-380; 1996, **32**, 187-189; 1997, **33**, 326-328 (*N-nicotinoyl, Trichophydine, Trichophysine, Muricatide*)
Uccello-Barretta, G. *et al., J.O.C.*, 1997, **62**, 827-835 (*R and S forms, synth, pmr*)
Laïb, T. *et al., Tetrahedron: Asymmetry*, 1998, **9**, 168-178 (*S-form, N-Ac, synth*)
Kawamoto, A.M. *et al., J.C.S. Perkin 1*, 2001, 1916-1928 (*N-benzyl, N-Boc, synth, ir, pmr, cmr*)
Becker, C.W. *et al., Synthesis*, 2005, 2549-2561 (*S-form, N-Me, resoln*)
Veum, L. *et al., Eur. J. Org. Chem.*, 2006, 1664-1671 (*N-Ac*)
Tanis, S. *et al., Tetrahedron*, 2006, **17**, 2154-2182 (*R-form, S-form, N-Me*)
Green, M.D. *et al., Chem. Biodiversity*, 2007, **4**, 118-128 (*N-di-Me, isol, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HNF000

1-Amino-4-phenyl-2,7-naphthyridine A-865

4-Phenyl-2,7-naphthyridin-1-amine, 9CI. ***Lophocladine B***

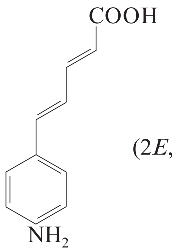


$C_{14}H_{11}N_3$ 221.261
Alkaloid from *Lophocladia* sp. Cytotoxic. Yellowish gum. λ_{max} 220 (log ϵ

4.01); 254 (log ε 4.02); 336 (log ε 3.89) (MeOH).

Gross, H. *et al., J. Nat. Prod.*, 2006, **69**, 640-644 (*isol, pmr, cmr, ms*)

5-(4-Aminophenyl)-2,4-pentadienoic acid A-866



(2*E*,4*E*)–*form*

$C_{11}H_{11}NO_2$ 189.213

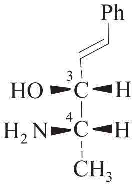
Prod. by *Streptomyces* sp. Tu 3946. Orange-brown solid. Mp 178°. Isol. as a mixt. of (2*E*,4*E*)- and (2*E*,4*Z*)-isomers.

Amide: 5-(4-Aminophenyl)-2,4-pentadienamide
$C_{11}H_{12}N_2O$ 188.229
Prod. by *Streptomyces* sp. Tu 3946. Yellow solid. Mp 205°. Mixt. of (2*E*,4*E*)- and (2*E*,4*Z*)-isomers.

[154824-88-1 , 154824-87-0 , 154824-83-6 , 154824-82-5]

Potterat, O. *et al., Helv. Chim. Acta*, 1994, **77**, 569 (*isol, synth*)

4-Amino-1-phenyl-1-penten-3-ol, 9CI A-867



(3*R*,4*S*)–*form*

$C_{11}H_{15}NO$ 177.246

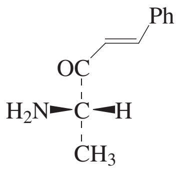
(1*E*,3*R*,4*S*)-*form*
Merucathine
[107673-74-5]
Alkaloid from *Catha edulis* (Celastraceae). Needles. Mp 129-130°. $[\alpha]^{20}_{D}$ +29.6 (c, 0.6 in MeOH).
Hydrochloride: [107673-75-6]
Mp 142-144°. $[\alpha]^{20}_{D}$ -5.2 (c, 0.4 in H_2O).

(1*E*,3*S*,4*S*)-*form*
Pseudomerucathine
[96861-89-1]
Alkaloid from *Catha edulis* (Celastraceae). Cryst. Mp 103-104°. $[\alpha]^{20}_{D}$ -15 (mixed solvent).
Hydrochloride: [107673-76-7]
Powder. Mp 194-196°. $[\alpha]^{20}_{D}$ -17.4 (c, 0.4 in H_2O).

Brenneisen, R. *et al., Planta Med.*, 1984, 531 (*isol, struct*)
Wolf, J.-P. *et al., Helv. Chim. Acta*, 1986, **69**, 918 (*struct, pmr, uv, cd, synth, abs config*)
Adam, W. *et al., Synthesis*, 1995, 1066 (*synth*)

4-Amino-1-phenyl-1-penten-3-one, 9CI A-868

Merucathinone



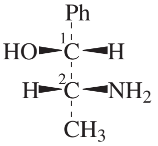
$C_{11}H_{13}NO$ 175.23

(1*E*,4*S*)-*form* [107638-80-2]
Alkaloid detected in *Catha edulis* (Celastraceae). Mp 144° dec. (as oxalate salt). $[\alpha]_D$ +7.5 (c, 0.85 in 2M HCl).

Wolf, J.-P. *et al., Helv. Chim. Acta*, 1986, **69**, 1498 (*synth, abs config, ir, uv, cd, pmr*)

2-Amino-1-phenyl-1-propanol A-869

α-(1-Aminoethyl)benzenemethanol, 9CI
[48115-38-4]



(1*R*,2*R*)-*form*

$C_9H_{13}NO$ 151.208

See also refs. under 2-(Methylamino)-1-phenyl-1-propanol, M-386. Anorectic agent, resolving agent. Log P 0.58 (calc).

(1*R*,2*R*)-*form*
D-threo-*form*. ***Nor-ψ-ephedrine***. *Norpseudoephedrine. Norisoephedrine. Cathine, INN*
[37577-07-4]
Found in "Ma Huang" and *Catha edulis* (Celastraceae) (Khat), used as a stimulant drink in Arab countries. Plates (MeOH). Mp 77°. $[\alpha]^{20}_{D}$ +33.14 (EtOH). Pharmacol. active isomer.
Hydrochloride: [53643-20-2]
Mp 180-181°. $[\alpha]^{20}_{D}$ +42.5 (H_2O).
▶ RC9350000
N-*Me:* see 2-(Methylamino)-1-phenyl-1-propanol, M-386

(1*S*,2*S*)-*form*
(-)-Nor-ψ-ephedrine. Katine
[492-39-7]
Synthetic. Mp 77.5-78°. $[\alpha]^{20}_{D}$ -32.64 (EtOH).
▶ LD_{50} (rat, orl) 1538 mg/kg. RC9100000
Hydrochloride: Mp 180-181°. $[\alpha]^{20}_{D}$ -42.7 (H_2O).
N-*Me:* see 2-(Methylamino)-1-phenyl-1-propanol, M-386
N,N-*Di-Me:* see 2-Dimethylamino-1-phenyl-1-propanol, D-738

(1*S*,2*R*)-*form*
(+)-Norephedrine
[37577-28-9]
Synthetic. Mp 52°. $[\alpha]^{27}_{D}$ +14.76 (EtOH).
Hydrochloride: [40626-29-7]
Mp 171-172°. $[\alpha]^{27}_{D}$ +33.4 (EtOH).
▶ RC3325000
N-*Me:* see 2-(Methylamino)-1-phenyl-1-propanol, M-386
N,N-*Dibutyl:* [114389-70-7]
$C_{17}H_{29}NO$ 263.422
Chiral catalyst, e.g. for enantioselective addn. of R_2Zn to aldehydes. Oil. Bp_2 170°. $[\alpha]^{22}_{D}$ -24.4 (c, 2 in hexane).

(1*R*,2*S*)-*form*
Norephedrine
[492-41-1]
Alkaloid from "Ma Huang", *Ephedra vulgaris* and *Catha edulis* (Ephedraceae, Celastraceae). Mp 51°. $[\alpha]_D$ -15 (EtOH).
▶ RC2275000
Hydrochloride: [3198-15-0]
Mp 171-172°. $[\alpha]^{20}_{D}$ -33.27 (H_2O).
▶ RC3240000
N-*Formyl:* **N-*Formylnorephedrine***
$C_{10}H_{13}NO_2$ 179.218
Alkaloid from leaves of *Catha edulis* (Celastraceae). Needles (Et_2O/hexane). Mp 72-73°. $[\alpha]^{25}_{D}$ -45 (c, 1.1 in $CHCl_3$).

(1*RS*, 2*RS*)-*form*
(±)-Nor-ψ-ephedrine
[54680-46-5]
Plates (petrol). Mp 77°.
Hydrochloride: [1485-15-0]
Mp 172-173°.
N-*Me:* see 2-(Methylamino)-1-phenyl-1-propanol, M-386

(1*RS*,2*SR*)-*form*
(±)-Norephedrine. ***Phenylpropanolamine, BAN, INN***. *Propadrine. Mydriatine*
[14838-15-4]
Adrenergic, vasoconstrictor. Nasal decongestant. Plates (H_2O). Mp 104-105° (101-101.5°). Log P 0.58 (calc).
▶ LD_{50} (rat, scu) 850 mg/kg. RC2625000
Hydrochloride: ***Phenylpropanolamine hydrochloride, USAN***
[154-41-6] Nasal decongestant. Sol. H_2O. Mp 194°. Component of Allerest, Demazin, Dimetapp, Sinarest.
▶ Hypertensive and CNS effects reported when used therapeutically. LD_{50} (rat, orl) 1490 mg/kg. Exp. teratogen. DN4200000
Complex with sulfonated styrene/divinylbenzene copolymer: ***Phenylpropanol amine polistirex, USAN***
Adrenergic, vasoconstrictor.
N-*Me:* see 2-(Methylamino)-1-phenyl-1-propanol, M-386

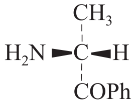
[36393-56-3 , 2153-98-2 , 54705-32-7 , 53631-70-2 , 700-65-2 , 4345-16-8 , 115651-77-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1273A; 1273B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 577A; 577B; 577C; 578A (*nmr*)
Wolfes, O. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1930, **268**, 81 (*isol*)
Leithe, W. *et al., Ber.*, 1932, **65**, 660 (*abs config*)
Hoover, F.W. *et al., J.O.C.*, 1947, **12**, 506 (*synth*)
Heacock, R.A. *et al., Can. J. Pharm. Sci.*, 1974, **9**, 64 (*pharmacol*)

Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9 (*occur*)
Baudet, M. *et al., Anal. Lett.*, 1979, **12**, 641 (*cmr*)
Kaufer, I. *et al., Anal. Profiles Drug Subst.*, 1983, **12**, 357
Al-Meshal, I.A. *et al., Phytochemistry*, 1986, **25**, 2241 (*N-Formylnorephedrine*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1277
Lasagna, L. *et al., Phenylpropanolamine: A Review*, Wiley, New York, 1988, (*book*)
Jackson, W.R. *et al., Aust. J. Chem.*, 1990, **43**, 2045 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1990, **15**, 219 (*use*)
Soai, K. *et al., J.O.C.*, 1991, **56**, 4264 (*synth, ir, pmr, use, deriv*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1222; 1252
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NNM000; NNN000; NNO000; NNM500; NNW500; PMJ500; NNV500; NNN500

2-Amino-1-phenyl-1-propanone, 9CI A-870

α-Aminopropiophenone. α-Benzoylethylamine. ***Cathinone, INN.*** *Norephedrone*
[5265-18-9]



(*R*)–*form*

$C_9H_{11}NO$ 149.192

Analgesic, anorectic, antinociceptive agent. Possesses psychostimulant props. Log P 0.84 (calc).

(R)-form [80096-54-4]
▶ UC0418990

Hydrochloride: [76333-53-4]
Cryst. (2-propanol/THF). Mp 189-190° dec. (175-177°). $[\alpha]_D^{23}$ +47.3 (c, 1 in H_2O).

(S)-form [71031-15-7]
Isol. from leaves of *Catha edulis* (Khat) (Celastraceae) which are chewed for narcotic effect. $[\alpha]_D^{26}$ -26.5 (c, 0.24 in CH_2Cl_2). Pharmacol. active enantiomer. Unstable except in dilute non-polar non-hydroxylic soln. Cathinone is the true alkaloid but is transformed in unfresh leaves to Ephedrine and Pseudoephedrine.
▶ UC0419000

Hydrochloride: [72739-14-1]
Cryst. (2-propanol/Et_2O). Mp 188-190° (176-178°). $[\alpha]_D^{21}$ -46.9 (c, 1 in H_2O).

Oxalate salt: [81626-17-7]
Fine cryst. (EtOH). Mp 173-175°. $[\alpha]_D^{25}$ -40.5 (c, 0.3 in MeOH).

(±)-form [75925-46-1]
Unstable solid. Mp 112-114°.

Hydrochloride: [42787-61-1]
Needles (EtOH/Et_2O). Mp 187°.

N-*Formyl:* [102831-14-1]
$C_{10}H_{11}NO_2$ 177.202
Cryst. (Me_2CO/hexane). Mp 93-96°.

N-*Ac:*
$C_{11}H_{13}NO_2$ 191.229
Cryst. (C_6H_6). Mp 90-91°.

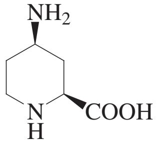
N-*Me: 2-Methylamino-1-phenyl-1-propanone. Ephedrone*
[5650-44-2]
$C_{10}H_{13}NO$ 163.219
Yellow oil. Bp_{11} 120-121°.

N-*Et:* [51553-17-4]
$C_{11}H_{15}NO$ 177.246
Shows anorexigenic activity in rats. Mp 196-198° (as hydrochloride). CAS no. refers to hydrochloride.

Gabriel, S. *et al., Ber.*, 1908, **41**, 1127 (*synth*)
Eberhard, A. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1915, **253**, 62
Kirchner, G. *et al., Annalen*, 1959, **625**, 104 (*synth*)
Schorno, X. *et al., Experientia*, 1979, **35**, 572 (*isol*)
Szendrei, K. *et al., Bull. Narc.*, 1980, **32**, 5 (*rev*)
Glennon, R.A. *et al., J. Med. Chem.*, 1980, **23**, 294 (*pharmacol*)
Berrang, B.D. *et al., J.O.C.*, 1982, **47**, 2643 (*resoln*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 12537
Kalix, P. *et al., Alcohol Alcohol.*, 1984, **19**, 319 (*pharmacol, use*)
Wolf, J.-P. *et al., Helv. Chim. Acta*, 1986, **69**, 918; 1498 (*synth, bibl*)
Muchowski, J.M. *et al., J.O.C.*, 1986, **51**, 3374 (*deriv*)
Farouz-Grant, F. *et al., J. Med. Chem.*, 1997, **40**, 1977-1981 (*synth, pmr*)

4-Amino-2-piperidinecarboxylic acid, 9CI A-871

4-Aminopipecolic acid, 8CI



(2*S*,4*R*)-*form*

$C_6H_{12}N_2O_2$ 144.173

(2S,4R)-form

Trifluoroacetate salt: [756486-08-5]
Solid. Mp 314° dec. $[\alpha]_D^{25}$ -5.1 (c, 0.75 in H_2O).

(2S,4S)-form
L-trans-form

Trifluoroacetate salt: [756486-10-9]
Solid. Mp 290° dec. $[\alpha]_D^{25}$ -10.4 (c, 0.64 in H_2O).

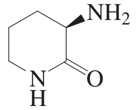
N-*Ac:* ***4-Acetamidopipecolic acid****. 2-Carboxy-4-acetylaminopiperidine*
[72015-68-0]
$C_8H_{14}N_2O_3$ 186.21
Alkaloid from leaves of *Calliandra haematocephala* (Fabaceae). Cryst. + ½ H_2O (Me_2CO aq.). $[\alpha]_D^{20}$ -6 (c, 0.20 in H_2O). $[\alpha]_D^{20}$ +0.5 (c, 0.196 in 2M HCl). Not correlated with the parent amine above due to scarcity of material. Incorr. descr. as (2*S*,4*R*) in the lit.

(-)-form
Present in *Strophanthus scandens* (Apocynaceae). Powder. Hygroscopic. Config. unknown.

Schenk, W. *et al., Naturwissenschaften*, 1961, **48**, 223 (*isol*)
Marlier, M. *et al., Phytochemistry*, 1979, **18**, 479 (*deriv*)
Machetti, F. *et al., Eur. J. Org. Chem.*, 2004, 2928-2935 (*2S,4R-form, 2S,4S-form, synth, pmr, cmr*)

3-Amino-2-piperidinone, 9CI A-872

Ornithine lactam. Cycloornithine
[1892-22-4]



(*R*)-*form*

$C_5H_{10}N_2O$ 114.147

(R)-form [88763-76-2]
Residue occurring in pyoverdins. Cryst. (EtOAc). Mp 85.5-87.5°.

N-tert-*Butyloxycarbonyl:* [221874-51-7]
$C_{10}H_{18}N_2O_3$ 214.264
Oil. $[\alpha]_D^{24}$ -57.4 (c, 1.07 in $CHCl_3$).

N-*Hydroxy; hydrochloride:* [37524-32-6]
Cryst. (MeOH/EtOH). Mp 208-215° dec. $[\alpha]_D^{24}$ -0.8 (c, 0.83 in H_2O).

(S)-form [34294-79-6]
Cryst. (EtOAc). Mp 42° Mp 86-87°. $[\alpha]_D^{25}$ -12.4 (c, 3.44 in $CHCl_3$). $[\alpha]_D^{25}$ -19.9 (dioxan).

Hydrochloride: [42538-31-8]
Mp 218-220° dec.

N^3-*Benzoyl:* [148824-28-6]
[3328-28-7 (L-form)]
$C_{12}H_{14}N_2O_2$ 218.255
Mp 170-172°.

N-*Hydroxy:* [40716-77-6]
$C_5H_{10}N_2O_2$ 130.146
Isol. from cultures of *Rhodotorula pilimanae*. Needles (MeOH/EtOH) (as hydrochloride). Mp 211-212° dec. (hydrochloride).

N^1-*4-Methylbenzenesulfonyl:* [20803-07-0]
Cryst. (MeOH). Mp 185-186°. $[\alpha]_D^{25}$ +60.9 (c, 2.04 in DMF).

(±)-form [4077-38-7]
Mp 42°. $Bp_{2.5}$ 125-135° lit. gives a pressure range.

N^3-*Ac:* [98336-92-6]
$C_7H_{12}N_2O_2$ 156.184
Needles ($CHCl_3$/Et_2O). Mp 187-188°.

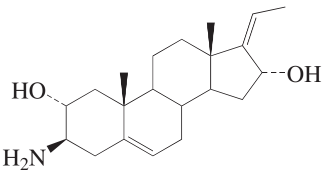
N-*Hydroxy; hydrochloride:*
[7438-77-9 (free base)]
Cryst. (EtOH). Mp 211-212°.

N-*Hydroxy,* N^3-*Ac:* [37524-31-5]
$C_7H_{12}N_2O_3$ 172.183
Cryst. (MeOH). Mp 203-205°.

Bergmann, M. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1926, **159**, 179-189 (*N³-Ac, synth*)
Emery, T.F. *et al., Biochemistry*, 1966, **5**, 3694-3701 (*S-form, hydroxy, synth*)
Isowa, Y. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 1464-1466 (*R-form, N-hydroxy, (±)-form, N-hydroxy N³-Ac, synth*)
Akers, H.A. *et al., Biochemistry*, 1973, **12**, 1006 (*isol, synth, S-form, N-hydroxy*)

Terashima, S. *et al., Tetrahedron*, 1973, **29**, 1487 (*synth*)
Merguro, H. *et al., Tet. Lett.*, 1975, 1309 (*cd*)
Pellegata, R. *et al., Synthesis*, 1978, 614-616 (*S-form, synth*)
Blade-Font, A. *et al., Tet. Lett.*, 1980, **21**, 2443 (*synth*)
Winter, W. *et al., Annalen*, 1983, 2021 (*synth*)
Miyamura, K. *et al., J.C.S. Dalton*, 1987, 1127 (*synth*)
Toshima, H. *et al., Tetrahedron*, 1999, **55**, 5793-5808 (*R-form, N-tert-butyloxycarbonyl*)
Abe, M. *et al., Bioorg. Med. Chem.*, 2005, **13**, 785-797 (*S-form, synth, pmr, cmr*)
Kubota, D. *et al., Bioorg. Med. Chem.*, 2006, **14**, 4158-4171 (*S-form, synth, pmr*)
Urbanczyk-Lipkowska, Z. *et al., Tetrahedron: Asymmetry*, 2007, **18**, 1254-1256 (*resoln, S-form*)

3-Aminopregna-5,17(20)-diene-2,16-diol A-873



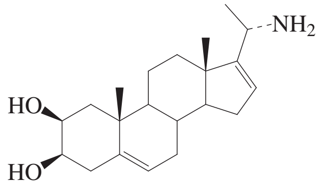
$C_{21}H_{33}NO_2$ 331.497

(2α,3β,16α,17Z)-form

N,N-*Di-Me: 3-(Dimethylamino)pregna-5,17(20)-diene-2,16-diol*. ***Kurchaline***
[6885-72-9]
$C_{23}H_{37}NO_2$ 359.551
Alkaloid from the leaves of *Holarrhena antidysenterica* (Apocynaceae). Cryst. (Me_2CO). Mp 185°. $[\alpha]_D$ -37 (c, 1 in $CHCl_3$).

Janot, M.M. *et al., Bull. Soc. Chim. Fr.*, 1966, 1212-1216 (*struct, ir, pmr, ms*)

20-Aminopregna-5,16-diene-2,3-diol A-874



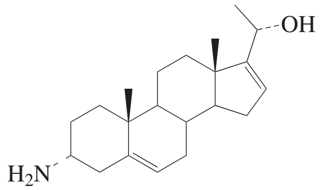
$C_{21}H_{33}NO_2$ 331.497

(2β,3β,20S)-form

3-Me ether, N^{20},N^{20}-*di-Me: 3-Methoxy-20-(dimethylamino)pregna-5,16-dien-2-ol.* ***Qasmine A***. *2-Hydroxy-*N*-methylsalignamine*
[657411-72-8]
$C_{24}H_{39}NO_2$ 373.578
Alkaloid from *Sarcococca saligna*. Acetylcholinesterase inhibitor. Yellow gum. $[\alpha]_D^{20}$ -26 (c, 0.02 in $CHCl_3$). Incorrect synonym assigned in ref. λ_{max} 206 (log ϵ 3.8) (MeOH).

Zaheer-ul-Haq, *et al., Bioorg. Med. Chem. Lett.*, 2003, **13**, 4375-4380 (*isol*)
Atta-ur-Rahman, *et al., Helv. Chim. Acta*, 2004, **87**, 439-448 (*isol, pmr, cmr, ms*)

3-Aminopregna-5,16-dien-20-ol A-875



$C_{21}H_{33}NO$ 315.498

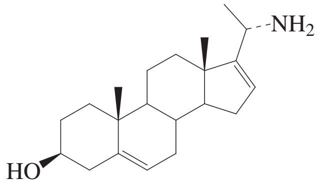
(3α,20S)-form

N-*Me:* ***Holadysamine***
[1433-91-6]
$C_{22}H_{35}NO$ 329.525
Minor alkaloid from the leaves of *Holarrhena antidysenterica* (Apocynaceae). Cryst. (hexane). Mp 173°. $[\alpha]_D$ -78 (c, 1 in $CHCl_3$).

N-*Me,* O,N-*di-Ac:* Mp 136°. $[\alpha]_D$ -74 (c, 1.3 in $CHCl_3$).

Janot, M.M. *et al., Bull. Soc. Chim. Fr.*, 1964, 2158-2166; 1966, 1212-1216 (*isol, struct, ir, pmr, ms*)

20-Aminopregna-5,16-dien-3-ol A-876



$C_{21}H_{33}NO$ 315.498

(3β,20S)-form

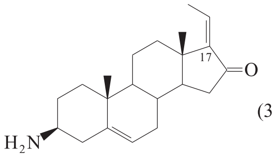
Me ether, N-*Me: 3-Methoxy-20-(methylamino)pregna-5,16-diene.* ***Salignamine***. *Qasmine B*
[657411-73-9]
$C_{23}H_{37}NO$ 343.551
Alkaloid from *Sarcococca saligna*. Cholinesterase and acetylcholinesterase inhibitor. Yellow gum. $[\alpha]_D^{20}$ -23 (c, 0.12 in $CHCl_3$). λ_{max} 202 (log ϵ 2.9) (MeOH).

Me ether, N-*Me,* N-*formyl:* ***N^{20}-Demethyl-N^{20}-formylsalonine B***
[657403-05-9]
$C_{24}H_{37}NO_2$ 371.562
Alkaloid from *Sarcococca saligna*. Cholinesterase inhibitor. Yellow gum. $[\alpha]_D^{20}$ -21 (c, 0.07 in MeOH). λ_{max} 237 (log ϵ 2.86) (MeOH).

Me ether, N,N-*di-Me: 20-(Dimethylamino)-3-methoxypregna-5,16-diene.* ***Salonine B***
[618852-70-3]
$C_{24}H_{39}NO$ 357.578
Alkaloid from *Sarcococca saligna*. Cholinesterase inhibitor. Powder. $[\alpha]_D^{20}$ -116 (c, 0.04 in MeOH). λ_{max} 206 (MeOH).

Zaheer-ul-Haq, *et al., Bioorg. Med. Chem. Lett.*, 2003, **13**, 4375-4380 (*N^{20}-Demethyl-N^{20}-formylsalonine B*)
Atta-ur-Rahman, *et al., Nat. Prod. Res.*, 2003, **17**, 235-241 (*Salonine B*)
Atta-ur-Rahman, *et al., Helv. Chim. Acta*, 2004, **87**, 439-448 (*Salignamine*)

3-Aminopregna-5,17(20)-dien-16-one A-877



(3β,17*E*)–*form*

$C_{21}H_{31}NO$ 313.482

(3β,17E)-form

N-*Me:* ***3-Methylaminopregna-5,17(20)-dien-16-one***
[113846-33-6]
$C_{22}H_{33}NO$ 327.509
Alkaloid from leaves of *Didymeles perrieri* (Didymelaceae). $[\alpha]_D$ -37 (c, 0.60 in EtOH).

(3β,17Z)-form

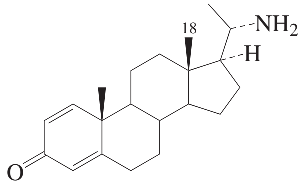
Alkaloid from leaves of *Didymeles perrieri* (Didymelaceae). $[\alpha]_D$ -63 (c, 0.41 in $CHCl_3$).

N-*Me:* [113846-32-5]
Alkaloid from leaves of *Didymeles perrieri* (Didymelaceae). $[\alpha]_D$ -16 (c, 0.68 in $CHCl_3$).

Sánchez, V. *et al., Bull. Soc. Chim. Fr.*, Part II, 1987, 877

20-Aminopregna-1,4-dien-3-one A-878

[77546-81-7]



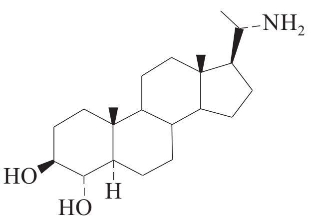
$C_{21}H_{31}NO$ 313.482

(20S)-form [78548-54-6]

N,N-*Di-Me:* ***20-(Dimethylamino)pregna-1,4-dien-3-one***
[91147-27-2]
$C_{23}H_{35}NO$ 341.536
Alkaloid from the stem bark of *Didymeles* cf *madagascariensis* (Didymelaceae). $[\alpha]_D$ +48 (c, 0.1 in $CHCl_3$).

Sánchez, V. *et al., Bull. Soc. Chim. Fr.*, Part II, 1984, 71; 1987, 877 (*isol, uv, cd, pmr, cmr, ms, struct*)
De, D. *et al., Steroids*, 1991, **56**, 189 (*synth*)

20-Aminopregnane-3,4-diol A-879



$C_{21}H_{37}NO_2$ 335.529

(3β,4α,5α,20*S*)-*form*

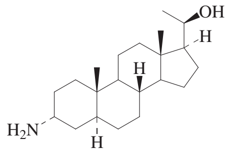
N,N-*Di-Me:* ***Terminaline***
[15112-49-9]
$C_{23}H_{41}NO_2$ 363.582
Alkaloid from *Pachysandra terminalis* and *Sarcococca hookeriana*. Cryst. Mp 243-244° (216-218°). $[\alpha]_D^{25}$ +115 (c, 0.04 in MeOH). λ_{max} 242 (ϵ 1000) (MeOH).

N,N-*Di-Me, Di*-O-*Ac:* Mp 202-204°. $[\alpha]_D$ +40 ($CHCl_3$).

Kikuchi, T. *et al., Tet. Lett.*, 1965, **24**, 1993-1999 (*isol, pmr, ms*)
Choudhary, M.I. *et al., Steroids*, 2005, **70**, 295-303 (*isol, pmr, cmr*)

3-Aminopregnan-20-ol A-880

3-Amino-20-hydroxypregnane



(3α,5α,20*R*)-*form*

$C_{21}H_{37}NO$ 319.529

(3α,5α,20*R*)-*form*

Isofuntumidine. Epifuntumidine
[516-52-9]
Cryst. (MeOH). Mp 172-173°. $[\alpha]_D$ -6.2 (c, 2.7 in $CHCl_3$).

(3α,5α,20*S*)-*form*

Funtumidine
[474-44-2]
Alkaloid from *Funtumia latifolia* (Apocynaceae). Hypocholesterolaemic agent. Shows antigonadotrophic, corticotrophic antiinflammatory and hypotensive activity. Respiratory stimulant. Mp 182°. $[\alpha]_D$ +10 (c, 1.5 in $CHCl_3$).
▶ TU4200000

(3α,5β,20*R*)-*form*

Cryst. (DMF). Mp 160-163°. $[\alpha]_D^{23.5}$ +14.4 (c, 1 in $CHCl_3$).

(3β,5α,20*R*)-*form*

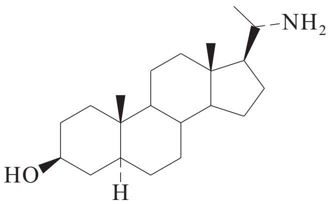
Cryst. Mp 172-174°. $[\alpha]_D^{21.5}$ +5.4 (c, 1 in $CHCl_3$).

(3β,5β,20*R*)-*form*

Cryst. (EtOAc). Mp 150-152°. $[\alpha]_D^{20}$ 0 (c, 1 in $CHCl_3$).

Janot, M.-M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1958, **246**, 3076; 1959, **248**, 982 (*ir, struct, Funtumidine*)
U.S. Pat., 1963, 3 098 082; *CA*, **59**, 11632d (*synth*)
Schmitt, J. *et al., Bull. Soc. Chim. Fr.*, 1964, 761 (*synth*)
Dodoun, H. *et al., Phytochemistry*, 1973, **12**, 923 (*Isofuntumidine*)

20-Aminopregnan-3-ol A-881



$C_{21}H_{37}NO$ 319.529

(3β,5α,20*S*)-*form*

Funtuphyllamine A
[667-71-0]
Alkaloid from *Funtumia africana* (Apocynaceae). Mp 173°. $[\alpha]_D$ +13 (c, 1.3 in $CHCl_3$).

N-*Ac:* ***Holacetine***
[60882-55-5]
$C_{23}H_{39}NO_2$ 361.567
Alkaloid from *Holarrhena antidysenterica* root bark (Apocynaceae). Mp 258°. $[\alpha]_D^{25}$ +6.9 (EtOH).

N-*Me: 20-Methylaminopregnan-3-ol.* ***Funtuphyllamine B***
[474-81-7]
$C_{22}H_{39}NO$ 333.556
Alkaloid from *Funtumia africana* and *Malouetia bequaertiana* (Apocynaceae). Mp 214°. $[\alpha]_D$ +24 ($CHCl_3$).

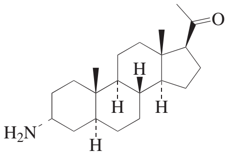
N,N-*Di-Me: 20-(Dimethylamino)pregnan-3-ol.* ***Funtuphyllamine C****. Sarcorucinine D*
[474-51-1]
$C_{23}H_{41}NO$ 347.583
Alkaloid from *Funtumia africana* (Apocynaceae). Also from *Sarcococca ruscifolia* (Buxaceae). Mp 172°. $[\alpha]_D$ +24 ($CHCl_3$).

N,N-*Di-Me,* O-*β*-D-*glucopyranoside:* ***Pachyaxioside A***
[128255-18-5]
$C_{29}H_{51}NO_6$ 509.725
Alkaloid from *Pachysandra axillaris.*

N,N-*Di-Me,* O-*(3-methyl-2-butenoyl):* ***O-β,β-Dimethylacrylylfuntuphyllamine C***
$C_{28}H_{47}NO_2$ 429.685
Alkaloid from *Sarcococca pruniformis* (Buxaceae). Mp 274-276°. $[\alpha]_D^{26}$ +10 ($CHCl_3$).

Černy, V. *et al., Coll. Czech. Chem. Comm.*, 1957, **22**, 76 (*synth*)
Janot, M.-M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1960, **250**, 2445 (*isol, ir, struct*)
Chatterjee, A. *et al., Chem. Ind. (London)*, 1966, 769 (*Dimethylacrylylfuntuphyllamine C*)
Demailly, G. *et al., Tet. Lett.*, 1975, 2471 (*synth*)
Rej, R.N. *et al., Phytochemistry*, 1976, **15**, 1173 (*Holacetine*)
Biesemans, M. *et al., Bull. Soc. Chim. Belg.*, 1985, **94**, 59 (*pmr, cmr, conformn*)
Qiu, M. *et al., Zhiwu Xuebao (Acta Bot. Sin.)*, 1989, **31**, 535; *CA*, **113**, ; 74724n (*Sarcorucinine D*)
Qiu, M. *et al., CA*, 1990, **113**, 55838m (*N,N-di-Me glucoside*)

3-Aminopregnan-20-one A-882



(3α,5α)-*form*

$C_{21}H_{35}NO$ 317.514

(3α,5α)-*form*

Funtumine
[474-45-3]
Alkaloid from *Funtumia latifolia*, *Holarrhena febrifuga* and *Holarrhena congolensis* (Apocynaceae).
Hypocholesterolaemic agent, shows antigonadotropic, corticotropic, antiinflammatory and hypotensive props. Respiratory stimulant. Mp 126°. $[\alpha]_D$ +95 (c, 1.7 in $CHCl_3$).
▶ LD_{50} (mus, ivn) 30 mg/kg. TU4375000

Hydrochloride: Mp 280°. $[\alpha]_D$ +60 (c, 0.67 in MeOH).

N-*Ac:* [4465-66-1]
Mp 240°.

N-*Me: 3-(Methylamino)pregnan-20-one.* **N-*Methylfuntumine***
[40855-51-4]
$C_{22}H_{37}NO$ 331.54
Alkaloid from *Holarrhena febrifuga* and *Sarcococca coriacea*. Yellow cryst.($CHCl_3$). Mp 129-130°. $[\alpha]_D^{20}$ +92 (c, 0.9 in $CHCl_3$). λ_{max} 202 (log ϵ 4.8) (MeOH).

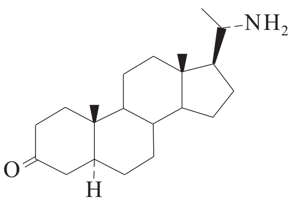
N,N-*Di-Me: 3-(Dimethylamino)pregnan-20-one.* **N,N-*Dimethylfuntumine***
[3022-47-7]
$C_{23}H_{39}NO$ 345.567
Alkaloid from *Holarrhena febrifuga* (Apocynaceae). Mp 128-130°. $[\alpha]_D^{20}$ +92 (c, 1.8 in $CHCl_3$).

(3β,5α)-*form*

Dihydroholaphyllamine
[2136-36-9]
[24202-19-5 (hydrochloride)]
Alkaloid from *Holarrhena floribunda* (Apocynaceae). Noncryst.

Janot, M.-M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1958, **246**, 3076; 1959, **248**, 982 (*isol, ir, struct*)
Leboeuf, M. *et al., Ann. Pharm. Fr.*, 1969, **27**, 217-218 (*Dihydroholaphyllamine*)
Boutigue, M.H. *et al., Bull. Soc. Chim. Fr.*, 1973, 750-753 (*synth, N-Methylfuntumine, N,N-Dimethylfuntumine*)
Dadoun, H. *et al., Phytochemistry*, 1973, **12**, 923-928 (*Funtumine, N-Methylfuntumine, N,N-Dimethylfuntumine*)
Kapnang, H. *et al., Tet. Lett.*, 1977, 3469-3472 (*N,N-Dimethylfuntumine, synth*)
Kalauni, S.K. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1423-1426 (*N-Methylfuntumine, pmr, cmr*)

20-Aminopregnan-3-one A-883



$C_{21}H_{35}NO$ 317.514

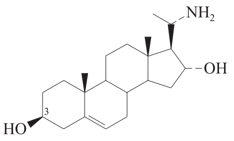
(5α,20S)-form
Wrightiamine B
[640266-39-3]
Alkaloid from the leaves of *Wrightia japonica*. Amorph. solid. $[\alpha]_D^{25}$ +5 (c, 0.04 in MeOH).

N-*Me: 20-(Methylamino)pregnan-3-one*. ***Funtumafrine B***
[474-82-8]
$C_{22}H_{37}NO$ 331.54
Alkaloid from the leaves of *Funtumia africana*. Mp 160°. $[\alpha]_D$ +43 (c, 1.2 in $CHCl_3$).

N,N-*Di-Me: 20-(Dimethylamino)pregnan-3-one*. ***Funtumafrine C***
[474-52-2]
$C_{23}H_{39}NO$ 345.567
Alkaloid from *Funtumia africana*, *Chonemorpha macrophylla* and *Sarcococca coriacea*. Cryst.($CHCl_3$). Mp 176° (174°). $[\alpha]_D^{25}$ +50 (c, 0.6 in $CHCl_3$). λ_{max} 202 (log ε 4.7) (MeOH).

Janot, M.M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1960, **250**, 2445-2447 (*isol, struct, synth*)
Banerji, J. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 346 (*isol*)
Kalauni, S.K. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1423-1426 (*Funtumafrine C, pmr, cmr*)
Kawamoto, S. *et al., Chem. Pharm. Bull.*, 2003, **51**, 737-739 (*Wrightiamine B*)

20-Aminopregn-5-ene-3,16-diol A-884



(3β,16α,20S)–*form*

$C_{21}H_{35}NO_2$ 333.513

(3β,16α,20S)-form

N-*Me: 20-(Methylamino)pregn-5-ene-3,16-diol*
[16378-59-9]
$C_{22}H_{37}NO_2$ 347.54
Mp 265°. $[\alpha]_D^{24}$ -69.9 (c, 0.5 in propanol).

N-*Me,* N*,3,16-tri-Ac:* Mp 214°. $[\alpha]_D^{30.5}$ -142 (c, 1 in $CHCl_3$).

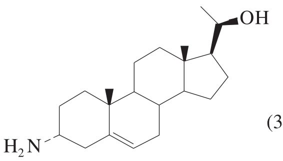
(3β,16β,20S)-form

3-Me ether, N,N-*di-Me: 20-(Dimethylamino)-3-methoxypregn-5-en-16-ol*. ***Pachyaximine B***
[128286-24-8]
$C_{24}H_{41}NO_2$ 375.593
Alkaloid from *Pachysandra axillaris* (Buxaceae).

Di-Me ether, N,N-*di-Me: 3,16-Dimethoxy-*N,N-*dimethylpregn-5-en-20-amine, 9CI. 20-(Dimethylamino)-3,16-dimethoxypregn-5-ene*. ***Sarcosaligmine***. *Sracosalgmine*
[873804-22-9]
$C_{25}H_{43}NO_2$ 389.62
Alkaloid from *Sarcococca saligna*. Solid. Mp 212-217°. $[\alpha]_D^{27}$ +77 (c, 0.44 in $CHCl_3$).

Schmitt, J. *et al., Bull. Soc. Chim. Fr.*, 1963, 2240-2248 (*N-Me, synth*)
Qui, M. *et al., Zhiwu Xuebao (Acta Bot. Sin.)*, 1989, **31**, 535-539; *CA*, **113**, 74724n (*Pachyaximine B*)
Naeem, I. *et al., CA*, 2005, **144**, 146530m (*Sarcosaligmine*)

3-Aminopregn-5-en-20-ol A-885



(3α,20R)-*form*

$C_{21}H_{35}NO$ 317.514

(3α,20R)-form
Holaminol
[28375-11-3]
Minor alkaloid from the leaves of *Holarrhena febrifuga* (Apocynaceae). Mp 205°. $[\alpha]_D$ -78.6 ($CHCl_3$). Phys. consts. for synthetic sample.

O,N-*Di-Ac:* Mp 226°. $[\alpha]_D^{20}$ -23.8 (c, 0.9 in $CHCl_3$).

(3β,20R)-form

N-*Me:* ***Holaphyllinol***
[5750-08-3]
$C_{22}H_{37}NO$ 331.54
Alkaloid from *Holarrhena floribunda* (Apocynaceae). Mp 226-227°. $[\alpha]_D$ -71 (c, 1.3 in $CHCl_3$).

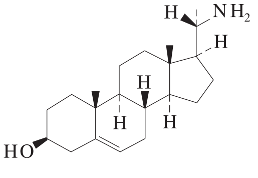
(3β,20S)-form

N-*Me:* ***Holaphyllidine***
[3837-07-8]
$C_{22}H_{37}NO$ 331.54
Alkaloid from *Holarrhena africana* (*Holarrhena floribunda*) (Apocynaceae).

Goutarel, R. *et al., Bull. Soc. Chim. Fr.*, 1962, 646 (*synth*)
Leboeuf, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1964, **259**, 3401 (*Holaphyllidine*)
Leboeuf, M. *et al., Ann. Pharm. Fr.*, 1969, **27**, 217 (*Holaphyllinol*)
Dadoun, H. *et al., Ann. Pharm. Fr.*, 1973, **31**, 237 (*isol, pmr, ms*)

20-Aminopregn-5-en-3-ol A-886

20-Amino-3-hydroxypregn-5-ene



(3β,20S)-*form*

$C_{21}H_{35}NO$ 317.514

(3β,20S)-form
Holafebrine
[5035-10-9]
Alkaloid from *Holarrhena febrifuga, Holarrhena mitis, Holarrhena crassifolia* and *Kibatalia arborea* (Apocynaceae). Mp 177°. $[\alpha]_D$ -61.5 (c, 0.85 in $CHCl_3$). $[\alpha]_D^{25}$ -66.6 (90% Py aq.).

O-*β-D-Glucopyranoside:* ***Conopharyngine***†
[7067-29-0]
$C_{27}H_{45}NO_6$ 479.656
Alkaloid from *Conopharyngia pachysiphon* (Apocynaceae). Hypotensive agent. Mp 285-288°.

O-*β-D-Glucopyranoside; hydrochloride:* Mp 259-260°. $[\alpha]_D^{25}$ -66.6 (90% Py aq.).

O,N-*Di-Ac:* Mp 250°. $[\alpha]_D$ -56.6 (c, 0.7 in $CHCl_3$).

N-*Me: 20-Methylaminopregn-5-en-3-ol*. ***Irehamine***
[7083-27-4]
$C_{22}H_{37}NO$ 331.54
Alkaloid from *Funtumia elastica, Funtumia latifolia* and *Dictyophleba lucida* (Apocynaceae). Mp 230°. $[\alpha]_D$ -33 (c, 0.9 in $CHCl_3$).

N,N-*Di-Me: 20-Dimethylaminopregn-5-en-3-ol*. ***Irehine***. *Buxomegine*
[2309-39-9]
$C_{23}H_{39}NO$ 345.567
Alkaloid from *Funtumia elastica* and *Buxus sempervirens*. Mp 174°. $[\alpha]_D^{25}$ +40 (c, 1.3 in $CHCl_3$). λ_{max} 204 (MeOH).

N,N-*Di-Me,* O-*β-D-glucopyranoside:* ***Pachyaxioside B***
[128255-19-6]
$C_{29}H_{49}NO_6$ 507.709
Alkaloid from *Pachysandra axillaris*.

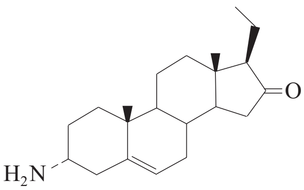
Me ether, N,N-*di-Me: 3-Methoxy-20-dimethylaminopregn-5-ene*. ***Pachyaximine A***
[128255-08-3]
[32164-75-3]
$C_{24}H_{41}NO$ 359.594
Alkaloid from *Pachysandra axillaris* and *Sarcococca pruniformis*. Needles. Mp 155° (152-153°). $[\alpha]_D^{30}$ -32 ($CHCl_3$). Alkaloid C from *S. pruniformis* originally assigned 3α-config.

Lucas, R.A. *et al., J.A.C.S.*, 1960, **82**, 5688 (*glucoside*)
Janot, M.-M. *et al., Bull. Soc. Chim. Fr.*, 1962, 285 (*isol, struct*)
Vetter, W. *et al., Bull. Soc. Chim. Fr.*, 1963, 1324 (*ms*)
Truong-Ho, M. *et al., Bull. Soc. Chim. Fr.*, 1963, 2332 (*derivs*)
Votický, Z. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 348 (*derivs*)
Robinson, C.H. *et al., Chem. Ind. (London)*, 1966, 377 (*pmr*)
Kohli, K.M. *et al., Phytochemistry*, 1971, **10**, 442 (*Alkaloid C*)
Einhorn, J. *et al., Phytochemistry*, 1972, **11**, 769 (*isol*)
Dadoun, H. *et al., Ann. Pharm. Fr.*, 1973, **31**, 237 (*isol*)
Qiu, M. *et al., Zhiwu Xuebao (Acta Bot. Sin.)*, 1989, **31**, 535; *CA*, **113**, 74724 (*Pachyaximine A*)
Qiu, M. *et al., CA*, 1990, **113**, 55838m (*glucoside*)

Atta-ur-Rahman, *et al., Nat. Prod. Res.*, 2003, **17**, 235-241 (*Alkaloid C*)

Babar, Z.U. *et al., Steroids*, 2006, **71**, 1045-1051 (*Irehine*)

3-Aminopregn-5-en-16-one A-887



$C_{21}H_{33}NO$ 315.498

3α-*form*

N-*Me: 3-Methylaminopregn-5-en-16-one.* ***Holadysine***

$C_{22}H_{35}NO$ 329.525

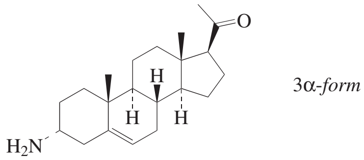
Alkaloid from the leaves of *Holarrhena antidysenterica* (Apocynaceae). Cryst. (hexane). Mp 120°. $[\alpha]_D$ -199 (c, 1.2 in $CHCl_3$).

N-*Me,* N-*Ac:*

Cryst. by subl. Mp 175°. $[\alpha]_D$ -163 (c, 1.3 in $CHCl_3$).

Janot, M.M. *et al., Bull. Soc. Chim. Fr.*, 1964, 2158; 1966, 1212 (*isol, struct, ir, pmr, ms*)

3-Aminopregn-5-en-20-one A-888



$C_{21}H_{33}NO$ 315.498

Log P 4.13 (uncertain value) (calc).

3α-*form*

Holamine

[28840-94-0]

Alkaloid from *Holarrhena curtisii* and *Holarrhena floribunda* and leaves of *Holarrhena febrifuga* (Apocynaceae). Antigonadotropic, corticotropic and antiinflammatory agent. Strong local anaesthetic. Respiratory depressant. Diuretic causing sodium retention. Cytotoxic and leishmanicidal agent. Cryst. (EtOAc). Mp 135-136°. $[\alpha]_D$ +23 (c, 0.88 in $CHCl_3$).

N-*Me: 3-Methylaminopregn-5-en-20-one.* ***Monomethylholamine***

[41567-48-0]

$C_{22}H_{35}NO$ 329.525

Alkaloid from leaves of *Holarrhena febrifuga* (Apocynaceae). Cryst. (Me_2CO). $[\alpha]_D^{20}$ +25 (c, 1 in $CHCl_3$). Constants refer to a synthetic sample.

N,N-*Di-Me: 3-Dimethylaminopregn-5-en-20-one.* ***Dimethylholamine***

[41515-65-5]

$C_{23}H_{37}NO$ 343.551

Alkaloid from leaves of *Holarrhena febrifuga* (Apocynaceae). Cryst. (Me_2CO). Mp 135°. $[\alpha]_D$ +18 (c, 1 in $CHCl_3$). Constants are for a synthetic sample.

15α-Hydroxy: 3-Amino-15-hydroxypregn-5-en-20-one. ***15-Hydroxyholamine***

[215595-78-1]

$C_{21}H_{33}NO_2$ 331.497

Alkaloid from *Holarrhena curtisii*. Cytotoxic and leishmanicidal agent. Amorph. $[\alpha]_D$ +47.2 (c, 0.23 in $CHCl_3$).

3β-*form*

Holaphyllamine

[7068-92-0 (hydrochloride)]

Alkaloid from *Holarrhena floribunda* and *Holarrhena crassifolia* (Apocynaceae). Antiinflammatory agent. Noncryst. Mp 300° dec. (260°) (as hydrochloride). $[\alpha]_D$ +33 (c, 0.68 in MeOH) (hydrochloride). Log P 4.13 (uncertain value) (calc).

N-*Me:* ***Holaphylline***

[562-02-7]

$C_{22}H_{35}NO$ 329.525

Alkaloid from *Holarrhena floribunda*, *Holarrhena febrifuga*, *Holarrhena congolensis* and *Holarrhena crassifolia* (Apocynaceae). Antigonatotropic, corticotropic and antiinflammatory agent. Respiratory depressant, diuretic. Mp 128°. $[\alpha]_D$ +23.7 ($CHCl_3$).

N-*Me,* N-*Ac:* [2842-66-2]

Mp 205-206°. $[\alpha]_D$ +16.7 (c, 1.2 in $CHCl_3$).

N,N-*Di-Me:* ***Dimethylholaphyllamine****.* *Methylholaphylline*

[6405-70-5]

$C_{23}H_{37}NO$ 343.551

Alkaloid from *Holarrhena floribunda* (Apocynaceae). Cryst. (MeOH). Mp 121°. $[\alpha]_D$ +30.5 (c, 0.86 in $CHCl_3$).

Janot, M.-M. *et al., Bull. Soc. Chim. Fr.*, 1959, 896-900 (*Holamine, Monomethylholamine, Dimethylholamine*)

Janot, M.-M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1960, **251**, 559-561 (*Holaphyllamine, Holamine*)

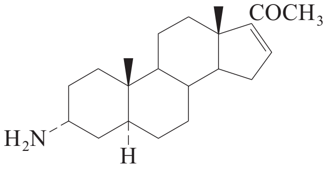
Goutarel, R. *et al., Bull. Soc. Chim. Fr.*, 1967, 4575-4582 (*synth, pmr*)

Einhorn, J. *et al., Phytochemistry*, 1972, **11**, 769-777 (*Holaphyllamine, Holaphylline*)

Dadoun, H. *et al., Phytochemistry*, 1973, **12**, 923-928 (*Holamine, Methylholamine, Dimethylholamine, isol, synth*)

Kam, T.-S. *et al., J. Nat. Prod.*, 1998, **61**, 1332-1336 (*Holamine, 15α-Hydroxyholamine, pmr, cmr*)

3-Aminopregn-16-en-20-one A-889



$C_{21}H_{33}NO$ 315.498

(3α,5α)-*form*

N-*Di-Me: 3-Dimethylaminopregn-16-en-20-one.* ***Sarcorucinine B***

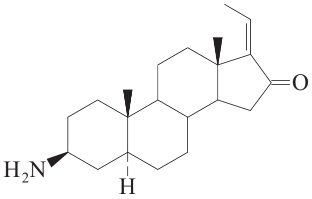
[143086-42-4]

$C_{23}H_{37}NO$ 343.551

Alkaloid from aerial parts of *Sarcococca ruscifolia* (Buxaceae).

Qiu, M. *et al., Yunnan Zhiwu Yanjiu*, 1991, **13**, 445; *CA*, **117**, 108079f (*isol, ir, pmr, ms*)

3-Aminopregn-17(20)-en-16-one A-890



$C_{21}H_{33}NO$ 315.498

(3β,5α,17*E*)-*form*

N-*Me:* ***3β-(Methylamino)pregn-17(20)-en-16-one***

[113846-34-7]

$C_{22}H_{35}NO$ 329.525

Alkaloid from the leaves of *Didymeles perrieri* (Didymelaceae). $[\alpha]_D$ -64 (c, 0.52 in $CHCl_3$).

N,N-*Di-Me: 3-(Dimethylamino)pregn-17(20)-en-16-one.* **E-*Salignone***

[204450-32-8]

$C_{23}H_{37}NO$ 343.551

Constit. of *Sarcococca saligna*. Oil. $[\alpha]_D^{25}$ -26 (c, 0.076 in $CHCl_3$). λ_{max} 242 (log ϵ 3.8) (MeOH).

(3β,5α,17*E*)-*form*

N,N-*Di-Me:* **Z-*Salignone***

[204450-33-9]

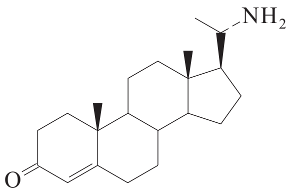
$C_{23}H_{37}NO$ 343.551

Constit. of *Sarcococca saligna*. Oil. $[\alpha]_D^{25}$ -46 (c, 0.086 in $CHCl_3$). λ_{max} 242 (log ϵ 3.7) (MeOH).

Sánchez, V. *et al., Bull. Soc. Chim. Fr.*, Part II, 1987, 877 (*isol, uv, ir, pmr, ms, cd, struct*)

Atta-ur-Rahman, *et al., Nat. Prod. Lett.*, 1998, **11**, 81-91 (*Salignones*)

20-Aminopregn-4-en-3-one A-891



$C_{21}H_{33}NO$ 315.498

(20*S*)-*form*

N-*Me: 20-Methylaminopregn-4-en-3-one.* ***4-Dehydrofuntumafrine B***

[16316-42-0]

$C_{22}H_{35}NO$ 329.525

Alkaloid from the leaves of *Didymeles madagascariensis.* $[\alpha]_D$ +91 (c, 0.72 in EtOH).

N,N-*Di-Me: 20-Dimethylaminopregn-4-en-3-one.* ***4-Dihydrofuntumafrine C****.* *Buxaprogestine*

[113762-72-4]

$C_{23}H_{37}NO$ 343.551
Alkaloid from the leaves of *Didymeles perrieri* and from leaves of *Buxus papilosa* (Buxaceae). $[\alpha]_D$ +49 (c, 1.8 in EtOH). $[\alpha]_D$ +26 (c, 1.78 in $CHCl_3$). Identity of the two samples not establ.

Sánchez, V. *et al., Bull. Soc. Chim. Fr.*, *Part II*, 1987, 877 (*isol, uv, ir, pmr, ms, cd, struct*)
Choudhary, M.I. *et al., Phytochemistry*, 1988, **27**, 271 (*Buxaprogestine*)

3-Aminopropanal, 9CI A-892

3-Aminopropionaldehyde, 8CI
[352-92-1]
$H_2NCH_2CH_2CHO$

C_3H_7NO 73.094
Liq. Bp_{12} 45-46°.

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 178°.

Di-Et acetal: 3,3-Diethoxy-1-propylamine. APEA
[41365-75-7]
$C_7H_{17}NO_2$ 147.217
Liq. Bp_{20} 68-70°.

N-*(3-Methylbutanoyl): 3-Methyl*-N-*(3-oxopropyl)butanamide, 9CI*. Diplocardia *Luciferin*
[58947-91-4]
$C_8H_{15}NO_2$ 157.212
Bioluminescent constit. of the earthworm *Diplocardia longa*. Oil.

N-*(3-Methylbutanoyl), 2,4-dinitrophenylhydrazone:*
Yellow cryst. Mp 174°.

N-tert-*Butyloxycarbonyl:* [58885-60-2]
$C_8H_{15}NO_3$ 173.211
Oil.

N-*Benzyloxycarbonyl:* [65564-05-8]
$C_{11}H_{13}NO_3$ 207.229
Mp 57-58°.

Albers, H. *et al., Ber.*, 1946, **79**, 623
Birkhofer, L. *et al., Chem. Ber.*, 1958, **91**, 2383
Ohtsuka, H. *et al., Biochemistry*, 1976, **15**, 1001 (*Luciferin*)
Geall, A.J. *et al., Tetrahedron*, 2000, **56**, 2449-2460 (*N-benzyloxycarbonyl, synth, pmr, cmr*)
Delfourne, E. *et al., J. Med. Chem.*, 2003, **46**, 3536-3545 (*N-tert-butyloxycarbonyl, synth, pmr, cmr*)

2-Amino-1,3-propanediol, 9CI, 8CI A-893

Serinol
[534-03-2]
$(HOCH_2)_2CHNH_2$

$C_3H_9NO_2$ 91.11
Mp 128°. Bp 264-265° $Bp_{0.06}$ 115-120°.

Hydrochloride: [73708-65-3]
Mp 104°.

Oxalate: [24070-20-0]
Hygroscopic cryst. Mp 202-203°.

N-*Ac:* [2655-79-0]
$C_5H_{11}NO_3$ 133.147
Mp 89-90°.

N-*(*tert-*Butyloxycarbonyl):* [125414-41-7]
$C_8H_{17}NO_4$ 191.227
Needles (hexane/EtOAc). Mp 84-85°.

N-*(2-Hydroxybenzoyl):* **N-*Salicyloyl-2-amino-1,3-propanediol***
$C_{10}H_{13}NO_4$ 211.217
Prod. by *Streptomyces hygroscopicus.* Antibacterial agent. Amorph. solid. λ_{max} 225 (log ϵ 4.32); 283 (sh) (log ϵ 3.54); 302 (sh) (log ϵ 3.5) (MeOH).

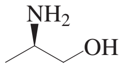
N-*(2-Hydroxybenzoyl), 1-Ac:*
$C_{12}H_{15}NO_5$ 253.254
Prod. by *Streptomyces hygroscopicus.* Antibacterial agent. Yellow amorph. solid. $[\alpha]_D^{25}$ -29 (c, 0.14 in MeOH). λ_{max} 228 (log ϵ 4.56); 282 (sh) (log ϵ 4.17); 301 (sh) (log ϵ 4.13) (MeOH).

Dibenzyl ether:
$C_{17}H_{21}NO_2$ 271.358
Oil.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 551B (*nmr*)
Den Otter, H.P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1938, **57**, 13 (*synth*)
Karrer, P. *et al., Helv. Chim. Acta*, 1948, **31**, 1617 (*oxalate, synth*)
Adkins, H. *et al., J.A.C.S.*, 1948, **70**, 3121 (*synth*)
Langenbeck, W. *et al., Naturwissenschaften*, 1955, **42**, 389 (*synth*)
Foster, A.B. *et al., J.C.S.*, 1958, 1890 (*synth*)
Szammer, J. *et al., Acta Chim. Acad. Sci. Hung.*, 1969, **61**, 417 (*synth*)
Japan. Pat., 1976, 76 67 788; *CA*, **85**, 157975 (*biosynth*)
Rai, B.L. *et al., J. Med. Chem.*, 1998, **41**, 3347-3359 (*dibenzyl ether*)
Neri, C. *et al., Adv. Synth. Catal.*, 2003, **345**, 835-848 (*tert-butyloxycarbonyl*)
Hossain, M.S. *et al., Phytochemistry*, 2004, **65**, 2147-2151 (*N-salicyloyl amides*)
Gu, K. *et al., Bioorg. Med. Chem.*, 2006, **14**, 1339-1347 (*synth, pmr, cmr*)

2-Amino-1-propanol, 9CI A-894

Alaninol. 2-Hydroxyisopropylamine
[78-91-1]



(*R*)-*form*

C_3H_9NO 75.11

(*S*)-*form* [2749-11-3]
Oil. Bp_{11} 72-73°. $[\alpha]_D^{20}$ +15.8.

N-*(2-Hydroxybenzoyl):* **N-*Salicyloyl-2-amino-1-propanol***
$C_{10}H_{13}NO_3$ 195.218
Prod. by *Streptomyces hygroscopicus.* Antibacterial agent. Amorph. solid. $[\alpha]_D^{25}$ -2.5 (c, 0.08 in MeOH).

[27646-78-2 , 92596-51-5 , 40916-69-6 , 40916-61-8 , 40916-73-2 , 57707-57-0 , 54490-98-1 , 15521-18-3]

Hossain, M.S. *et al., Phytochemistry*, 2004, **65**, 2147-2151 (*N-salicyloyl amide*)

(3-Aminopropoxy)guanidine, 9CI A-895

γ-Guanidinooxypropylamine
[97091-01-5]
$HN{=}C(NH_2)NHOCH_2CH_2CH_2NH_2$

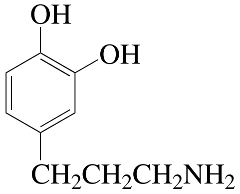
$C_4H_{12}N_4O$ 132.165
Constit. of *Canavalia gladiata* (swordbean) and *Wisteria floribunda.*

Hamana, K. *et al., Biochem. Biophys. Res. Commun.*, 1985, **129**, 46 (*isol*)

Matsuzaki, S. *et al., Phytochemistry*, 1990, **29**, 1311 (*isol*)

4-(3-Aminopropyl)-1,2-benzenediol, 9CI A-896

3-(3,4-Dihydroxyphenyl)-1-propylamine. Homodopamine
[52336-45-5]



$C_9H_{13}NO_2$ 167.207

Hydrobromide: [52336-30-8]
Cryst. (2-propanol). Mp 156-158°.

Di-Me ether: 3,4-Dimethoxybenzenepropanamine, 9CI. 3-(3,4-Dimethoxyphenyl)propylamine, 8CI
[14773-42-3]
$C_{11}H_{17}NO_2$ 195.261
Constit. of *Piper arboricola*. Bp_{15} 158-161°.

Di-Me ether, hydrochloride: [59734-58-6]
Cryst. (MeOH/EtOAc). Mp 166-167°.

Di-Me ether, picrate:
Cryst. (EtOH). Mp 145-146°.

Benington, F. *et al., J.O.C.*, 1956, **21**, 1545-1546 (*synth, di-Me ether*)
Winn, M. *et al., J. Med. Chem.*, 1975, **18**, 434-437 (*synth*)
Ho, C.F. *et al., CA*, 1981, **95**, 138470w (*isol, deriv*)

N-(3-Aminopropyl)-1,5-pentanediamine, 9CI A-897

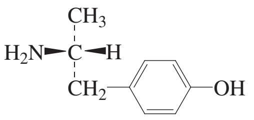
N-*(3-Aminopropyl)cadaverine. 1,9-Diamino-4-azanonane. 1,5,11-Triazaundecane.* as-*Homospermidine*
[56-19-9]
$H_2NCH_2(CH_2)_3CH_2NHCH_2CH_2CH_2NH_2$

$C_8H_{21}N_3$ 159.274
Isol. from *Hydrogenobacter halophilus* and *Paracoccus* sp. Cryst. (EtOH) (as trihydrochloride). Mp 258-259° (trihydrochloride). Bp 94-95°.

Mervyn, I. *et al., J. Med. Chem.*, 1964, **7**, 710-716 (*synth*)
Hamana, K. *et al., Biochem. J.*, 1992, **284**, 741-747 (*isol*)

4-(2-Aminopropyl)phenol, 9CI, 8CI A-898

1-(4-Hydroxyphenyl)-2-propylamine. p-*β-Aminopropylphenol.* ***Hydroxyamfetamine, INN****. Hydroxyamphetamine, BAN. Methyltyramine. Norpholedrine. Norveritol. Oxamphetamine. Paredrinex*
[103-86-6]



(*R*)-*form*

$C_9H_{13}NO$ 151.208

Sympathomimetic and mydriatic drug. Amphetamine metab. Log P 0.92 (calc).

▶SJ6475010

(R)-form [1518-89-4]
Mp 109-111.5°. $[M]_D^{20}$ -56° (c, 0.02 in EtOH).

Me ether: [50505-80-1]
$C_{10}H_{15}NO$ 165.235
Needles (EtOH/Et_2O) (as hydrochloride). Mp 251-253° dec. (hydrochloride). $[\alpha]_D^{25}$ -23.2 (c, 2.03 in H_2O). CAS no. refers to hydrochloride.

(S)-form [1693-66-9]
Mp 110-111.5°. $[M]_D^{20}$ + 59° (c, 0.02 in EtOH).

(±)-form [1518-86-1]
Alkaloid from *Acacia rigidula*. Cryst. (C_6H_6). Mp 125°.

Hydrobromide: ***Hydroxyamphetamine hydrobromide, USAN****. Mycadrine. Paredrine. Pedrolon*
[140-36-3]
Cryst. (EtOH/Et_2O). Mp 171-172°.

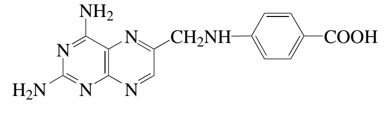
▶SJ6650000

Me ether: 4-Methoxy-α-methylbenzeneethanamine. 1-(4-Methoxyphenyl)-2-propylamine. 4-Methoxyamphetamine
[23239-32-9]
[64-13-1]
$C_{10}H_{15}NO$ 165.235
Alkaloid from *Acacia rigidula*.
Liq. Mp 210° (as hydrochloride). Bp_{14} 141°.

Mannich, C. *et al., Ber.*, 1910, **43**, 189 (*synth*)
Hoover, F.W. *et al., J.O.C.*, 1947, **12**, 501 (*synth*)
Dirkx, I.P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1964, **83**, 535 (*ord*)
v. Dijk, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1965, **84**, 521 (*resoln*)
Sever, P.S. *et al., Biochem. Soc. Trans.*, 1973, **1**, 1158 (*metab*)
Hahn, W.E. *et al., Acta Pol. Pharm.*, 1979, **36**, 259 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1246
Clement, B.A. *et al., Phytochemistry*, 1998, **49**, 1377-1380 (*Me ether, isol*)
Kohno, H. *et al., Synth. Commun.*, 1998, **28**, 1935-1945 (*Me ether*)

Aminopteroic acid A-899

4-[[(2,4-Diamino-6-pteridinyl)methyl]amino]benzoic acid, 9CI. p-*[*N*-2,4-Diamino-6-pteridyl]methylaminobenzoic acid*
[36093-85-3]



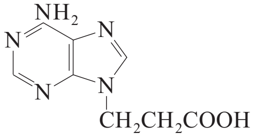
$C_{14}H_{13}N_7O_2$ 311.302
Parent acid present in Aminopterin.

N^{ar}*-Me: 4-[[(2,4-Diamino-6-pteridinyl)methyl]methylamino]benzoic acid*
[19741-14-1]
$C_{15}H_{15}N_7O_2$ 325.329
Orange powder. Mp > 300°.

Sato, H. *et al., Nippon Kagaku Kaishi*, 1951, **72**, 866; *CA*, **47**, 5946
U.S. Pat., 1951, 2 568 597; *CA*, **46**, 5094
Venditti, J.M. *et al., Cancer Res.*, 1960, **20**, 691
Elliott, R.D. *et al., J.O.C.*, 1970, **35**, 1676-1680 (*N-Me*)
Piper, J.R. *et al., J.O.C.*, 1977, **42**, 208

6-Amino-9*H*-purine-9-propanoic acid, 9CI A-900

3-(9-Adeninyl)propionic acid
[4244-47-7]



$C_8H_9N_5O_2$ 207.191
Isol. from *Lentinus edodes* (shiitake). Exhibits anticholesteraemic activity. Mp 277-278° dec. λ_{max} 262 (ε 14400) (0.1*N* NaOH). λ_{max} 259 (ε 13800) (0.1*N* HCl).

Me ester: [70259-15-3]
$C_9H_{11}N_5O_2$ 221.218
Cryst. (Et_2O/MeOH). Mp 182-183°.

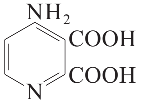
Et ester: [7083-40-1]
$C_{10}H_{13}N_5O_2$ 235.245
Solid. Mp 167-168°.

Nitrile: 6-Amino-9-(2-cyanoethyl)purine
[4244-45-5]
$C_8H_8N_6$ 188.191
Solid (H_2O). Mp 258-261° (245-247°).

Lira, E.P. *et al., J.O.C.*, 1966, **31**, 2188-2191 (*acid, nitrile, synth*)
Chakraborti, S.K. *et al., Indian J. Chem.*, 1969, **7**, 426 (*synth*)
Saito, Y. *et al., Tet. Lett.*, 1970, 4863 (*isol, struct, synth*)
Holy, A. *et al., Coll. Czech. Chem. Comm.*, 1978, **43**, 3444-3465 (*synth*)
Poritere, S.E. *et al., Khim. Geterotsikl. Soedin.*, 1982, 539-541; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1982, 415-417 (*nitrile*)

4-Amino-2,3-pyridinedicarboxylic acid, 9CI A-901

[122475-55-2]

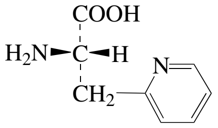


$C_7H_6N_2O_4$ 182.135
Isol. from fruit bodies of the poisonous mushroom *Clitocybe acromelalga*. Cryst. (H_2O). Sol. H_2O, MeOH; poorly sol. Me_2CO, hexane. λ_{max} 262 (ε 9550) (0.1*N* HCl) (Derep). λ_{max} 245 (sh) (ε 8710); 290 (ε 2090) (H_2O at pH 11) (Derep). λ_{max} 265 (ε 9120) (H_2O pH 7) (Derep). λ_{max} 252 (ε 10000) (MeOH) (Berdy). λ_{max} 265 (ε 9800); 290 (ε 2080) (H_2O) (Berdy).

Hirayama, F. *et al., Phytochemistry*, 1989, **28**, 1133 (*isol, uv, ir, pmr, cmr, ms, synth, struct*)

2-Amino-3-(2-pyridinyl)propanoic acid A-902

α-Amino-2-pyridinepropanoic acid, 9CI. 3-(2-Pyridinyl)alanine. Antibiotic SF 2538. SF 2538
[17407-39-5]
[37535-52-7]



(*S*)-*form*

$C_8H_{10}N_2O_2$ 166.179

(S)-form [37535-51-6]
[120191-52-8]
Prod. by *Streptomyces albus*. Cryst. Sol. H_2O; poorly sol. Me_2CO, hexane. $[\alpha]_D$ -33.6 (H_2O). Incorrectly indexed in CA. λ_{max} 254 (ε 3720); 260 (ε 4170); 266 (ε 3100) (H_2O). λ_{max} 254 (ε 3720); 260 (ε 4170); 266 (ε 3100) (H_2O) (Berdy). λ_{max} 261 (ε 7600) (HCl) (Berdy).

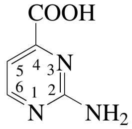
(±)-form [17407-44-2]
Cryst. (EtOH aq.). Mp 209-212° (209-210°).

[177164-50-0 , 169547-60-8 , 33715-92-3 , 172927-00-3 , 163513-22-2 , 33560-87-1]

Slater, G. *et al., Tetrahedron*, 1967, **23**, 2823-2828 (*synth*)
Watanabe, H. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1634-1638 (*synth*)
Veselova, L.N. *et al., Zh. Obshch. Khim.*, 1972, **42**, 1123-1125; 1973, **43**, 1637-1640 (*synth, resoln*)
Iwata, M. *et al., CA*, 1989, **110**, 169903x (*isol*)
Zhao, J.S. *et al., Yaoxue Xuebao*, 1994, **29**, 558-560; *CA*, **122**, 10513w (*synth*)

2-Amino-4-pyrimidinecarboxylic acid A-903

[2164-65-0]



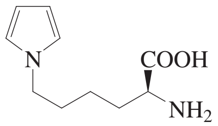
$C_5H_5N_3O_2$ 139.113
Constit. of *Lathyrus tingitanus* seeds. Precursor of the pyrimidine moiety of Lathyrine. Fine needles (H_2O). Mp 265° dec Mp 285° dec.

Nitrile: 2-Amino-4-cyanopyrimidine
[36314-98-4]
$C_5H_4N_4$ 120.113
Mp 222° dec.

Matsukawa, T. *et al., Yakugaku Zasshi*, 1952, **72**, 909; *CA*, **47**, 6425d (*synth*)
Whitlock, B.J. *et al., J.O.C.*, 1965, **30**, 115 (*synth, uv*)
Brown, E.C. *et al., Phytochemistry*, 1996, **42**, 61 (*occur*)
Doláková, P. *et al., Heterocycles*, 2007, **71**, 1107-1115 (*nitrile*)

α-Amino-1*H*-pyrrole-1-hexanoic acid, 9CI A-904

N$^{\epsilon}$-Pyrrolylnorleucine. Pyrrole-1-norleucine. 1-(5′-Amino-5′-carboxypentyl)pyrrole



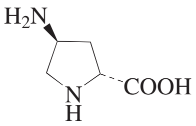
$C_{10}H_{16}N_2O_2$ 196.249

(S)-form
L-form
[156539-32-1]
Secondary lipid peroxidation prod. derived from L-lysine and 4,5-epoxy-2-alkenols. Widely distributed in fresh foodstuffs, e.g. meats, fish, vegetables and nuts. Characterised spectroscopically.

Chiang, G.H. *et al., J. Agric. Food Chem.*, 1988, **36**, 506-509 (*hplc, occur*)
Zamora, R. *et al., Lipids*, 1994, **29**, 243-249; 1995, **30**, 477-483 (*synth, detn, pmr, cmr*)
Zamora, R. *et al., Biochim. Biophys. Acta*, 1995, **1258**, 319-327 (*formn*)
Hidalgo, F.J. *et al., J. Agric. Food Chem.*, 1995, **43**, 1023-1028 (*occur, formn*)
Zamora, R. *et al., J. Agric. Food Chem.*, 1999, **47**, 1942-1947 (*occur*)

4-Amino-2-pyrrolidinecarboxylic acid A-905

4-Aminoproline, 9CI
[3285-76-5]



(2R,4S)-form

$C_5H_{10}N_2O_2$ 130.146

(2R,4S)-form
(+)-trans-*form*
Prod. by *Ascochyta caulina*. Phytotoxin. $[\alpha]_D^{21}$ +47.2 (c, 0.4 in H_2O).

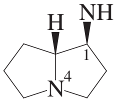
(2S,4R)-form
(-)-trans-*form*
[16257-88-8]
Prisms. Mp 229-230° dec. $[\alpha]_D^{21}$ -57.8 (H_2O).
Hydrochloride (1:2): [16257-89-9]
Mp 257-258°.
N-tert-*Butyloxycarbonyl:* [132622-69-6]
$C_{10}H_{18}N_2O_4$ 230.263
Solid. Mp 240-241° dec. $[\alpha]_D$ -35.9 (c, 1.0 in H_2O).
N^1-(4-Methylbenzenesulfonyl): [16257-87-7]
$C_{12}H_{16}N_2O_4S$ 284.335
Prisms (EtOH aq.). Mp 275-276° dec. $[\alpha]_D^{20}$ -62.7 (EtOH aq.).

(2S,4S)-form
(-)-cis-*form*
[16257-83-3]
Prisms (EtOH aq.). Mp 191-193° dec. $[\alpha]_D^{20}$ -57.4 (H_2O). Unstable.
Hydrochloride (1:2): [16257-84-4]
Mp 247°.
N-tert-*Butyloxycarbonyl:* [132622-66-3]
Solid. Mp 225-228° dec. $[\alpha]_D^{20}$ +21 (c, 0.24 in H_2O).
N^1-(4-Methylbenzenesulfonyl): [16257-82-2]
Needles (EtOH aq.). Mp 284-285° dec. $[\alpha]_D^{20}$ -72 (EtOH aq.).

Andreatta, R.H. *et al., Aust. J. Chem.*, 1967, **20**, 1493; 2701 (*synth, pmr*)
Webb, T.R. *et al., J.O.C.*, 1991, **56**, 3009-3016 (*N-Boc*)
Evidente, A. *et al., Phytochemistry*, 2000, **53**, 231-237 (*isol, pmr, cmr*)
Fisher, A. *et al., J. Med. Chem.*, 2006, **49**, 307-317 (*N-Boc*)

1-Aminopyrrolizidine A-906

*Hexahydro-1*H*-pyrrolizin-1-amine*
[170442-12-3]



$C_7H_{14}N_2$ 126.201

(1S,7aR)-form
(-)-cis-*form*
Waxy solid. $[\alpha]_D^{20}$ -24.1 (c, 5.5 in MeOH).
N^1-(2-Methylbutanoyl): ***Laburnamine***
[2072-58-4]
$C_{12}H_{22}N_2O$ 210.319
Alkaloid from the seeds of *Cytisus laburnum*. Mp 125-127°.
*N^1-(4-Methoxy-*E*-cinnamoyl):* ***Absouline***
[112513-33-4]
$C_{17}H_{22}N_2O_2$ 286.373
Alkaloid from *Hugonia oreogena* and *Hugonia penicillanthemum*. Cryst. (Me_2CO). Mp 186°. $[\alpha]_D$ +56 (c, 1 in EtOH).
*N^1-(4-Methoxy-*E*-cinnamoyl), N^4-oxide:* ***Absouline* N-*oxide***
[112494-54-9]
$C_{17}H_{22}N_2O_3$ 302.372
From *Hugonia oreogena* and *Hugonia penicillanthemum*. Amorph. $[\alpha]_D$ +13 (c, 0.9 in EtOH).
*N^1-(4-Methoxy-*Z*-cinnamoyl):* ***Isoabsouline***
[112513-34-5]
$C_{17}H_{22}N_2O_2$ 286.373
From *Hugonia oreogena* and *Hugonia penicillanthemum*. Amorph.
*N^1-(4-Methoxy-*Z*-cinnamoyl), N^4-oxide:* ***Isoabsouline* N-*oxide***
[112494-55-0]
$C_{17}H_{22}N_2O_3$ 302.372
From *Hugonia oreogena* and *Hugonia penicillanthemum*. Amorph.

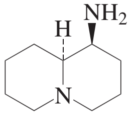
(1RS,7aRS)-form
(±)-trans-*form*
[141197-03-7]
Amorph. solid.

(1RS,7aSR)-form
(±)-cis-*form*
[145511-58-6]
Characterised spectroscopically.
[66393-07-5 , 66393-06-4]

Neuner-Jehle, N. *et al., Monatsh. Chem.*, 1965, **96**, 321-338 (*Laburnamine*)
Ikhiri, K. *et al., J. Nat. Prod.*, 1987, **50**, 626-630 (*Absouline, Absouline N-oxide, Isoabsouline, Isoabsouline N-oxide*)
Christine, C. *et al., Tetrahedron*, 2000, **56**, 1837-1850 (*SR-form, RS,RS-form, RS,SR-form, synth, pmr, cmr*)
Giri, N. *et al., J.O.C.*, 2004, **69**, 7303-7308 (*(-)-cis-form*)
Vargas-Sanchez, M. *et al., Org. Lett.*, 2005, **7**, 5861-5864 (*synth*)
Matos, M.N. *et al., Tetrahedron*, 2005, **61**, 1221-1244 (*Laburnamine, synth*)

1-Aminoquinolizidine A-907

*Octahydro-2*H*-quinolizin-1-amine, 9CI*
[80220-52-6]



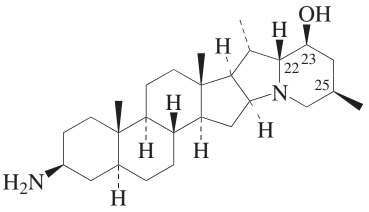
$C_9H_{18}N_2$ 154.255

(1S,9aS)-form
N^1-Ac: 1-Acetamidoquinolizidine. ***Epiquinamide****. Alkaloid 196. Quinolizidine 196*
[616235-95-1]
$C_{11}H_{20}N_2O$ 196.292
Alkaloid from the skin extracts of the frog *Epipedobates tricolor*. Nicotinic agonist. $[\alpha]_D^{20}$ +19 (c, 0.9 in $CHCl_3$).

Fitch, R.W. *et al., J. Nat. Prod.*, 2003, **66**, 1345-1350 (*isol, pmr, cmr*)
Kanakubo, A. *et al., Bioorg. Med. Chem. Lett.*, 2006, **16**, 4648-4651 (*synth*)
Huang, P.-Q. *et al., Org. Lett.*, 2006, **8**, 1435-1438 (*synth*)
Suyama, T.L. *et al., Org. Lett.*, 2006, **8**, 4541-4543 (*synth*)
Tong, S.T. *et al., Tet. Lett.*, 2006, **47**, 5017-5020 (*synth*)
Voituriez, A. *et al., Org. Lett.*, 2007, **9**, 4705-4708 (*synth*)
Wijdeven, M.A. *et al., Org. Lett.*, 2008, **10**, 4001-4003 (*synth, abs config*)

3-Aminosolanidan-23-ol, 9CI A-908

3-Amino-23-hydroxysolanidane



(3β,5α,22*R*,23*S*,25*R*)-*form*

$C_{27}H_{46}N_2O$ 414.673

(3β,5α,22R,23S,25R)-form
Solanogantine
[63785-19-3]
Alkaloid from leaves of *Solanum giganteum* (Solanaceae). Glass. Unusual 22β*H*-config., first natural 3-aminosolanidane.
N,O-Di-Ac: Mp 219-221° dec. $[\alpha]_D$ +27.2 ($CHCl_3$).

N,N-*Di-Me:* Mp 111-112°. $[\alpha]_D$ +41.3 ($CHCl_3$).

(3β,5α,22S,23S,25R)-form
Solanogantamine
[72075-33-3]
Alkaloid from *Solanum giganteum* and *Solanum vegum* (major alkaloid) (Solanaceae). Plates (MeOH/MeCN). Mp 180°. $[\alpha]_D$ +35 ($CHCl_3$).

N,O-*Di-Ac:*
Needles (Me_2CO aq.). Mp 229-231°. $[\alpha]_D$ +11 ($CHCl_3$).

N,N-*Di-Me:* Mp 207-210°. $[\alpha]_D$ +50 ($CHCl_3$).

(3α,5α,22S,23S,25R)-form
Isosolanogantamine
[72075-53-7]
Alkaloid from *Solanum giganteum* (Solanaceae). Flakes ($CHCl_3$/petrol). Mp 252-254°. $[\alpha]_D$ +31 ($CHCl_3$).

N,O-*Di-Ac:*
Cryst. (Me_2CO). Mp 257-259°. $[\alpha]_D$ +35.5 ($CHCl_3$).

N,N-*Di-Me:*
Flakes (MeOH). Mp 200-203°. $[\alpha]_D$ +41 ($CHCl_3$).

(3β,5α,22S,23S,25S)-form
Solanopubamine
[97858-53-2]
Alkaloid from the aerial parts of *Solanum pubescens* (Solanaceae). Needles (Me_2CO/MeOH). Mp 263°. $[\alpha]_D$ +30.5 (MeOH).

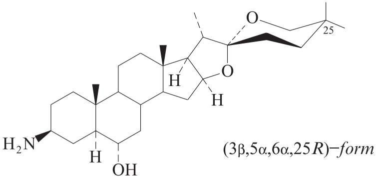
N-*Formyl:* ***Solanopubamide A***
[105705-84-8]
$C_{28}H_{46}N_2O_2$ 442.684
Alkaloid from the aerial parts of *Solanum pubescens* (Solanaceae). Needles (MeOH). Mp 209-210°. $[\alpha]_D$ +26.1 ($CHCl_3$).

N-*Ac:* ***Solanopubamide B***
[105814-55-9]
$C_{29}H_{48}N_2O_2$ 456.71
Alkaloid from the aerial parts of *Solanum pubescens* (Solanaceae). Needles (MeOH). Mp 255-256°. $[\alpha]_D$ +40 ($CHCl_3$).

N,O-*Di-Ac:*
Needles (MeOH). Mp 232°.

Pakrashi, S.C. *et al., Tet. Lett.*, 1977, 645 (*isol, ms, pmr, struct, synth*)
Pakrashi, S.C. *et al., J. Indian Chem. Soc.*, 1978, **55**, 1109 (*isol, ir, pmr*)
Chakravarty, A.K. *et al., J.C.S. Perkin 1*, 1984, 467 (*config*)
Krishna, G.N. *et al., Phytochemistry*, 1985, **24**, 1369 (*Solanopubamine*)
Kumari, G.N.K. *et al., Phytochemistry*, 1986, **25**, 2003 (*Solanopubamides*)

3-Aminospirostan-6-ol, 9CI A-909



$C_{27}H_{45}NO_3$ 431.657

(3β,5α,6α,25R)-form
Isojuripidine
[23656-00-0]
Alkaloid from *Solanum asterophorum* and *Solanum paniculatum*. Cryst. (MeOH). Mp 204-205° (200°). $[\alpha]_D$ -47 (c, 0.013 in $CHCl_3$).

O,N-*Di-Ac:* Mp 153-154°.

Glycoside: ***Isojuripine***
$C_{33}H_{55}NO_8$ 593.799
From *Solanum paniculatum* (Solanaceae). Mp 162-171°. $[\alpha]_D$ -20 (Py). β-Glycoside of undetd. struct.

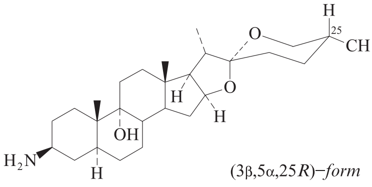
(3β,5α,6α,25S)-form
Juripidine
[89945-92-6]
Alkaloid from roots of *Solanum hispidum*.

N-*Ac:*
Cryst. (MeCN). Mp 260-262°. $[\alpha]_D$ -78.12 (c, 0.32 in $CHCl_3$).

N,O-*Di-Ac:* Mp 264-266°. $[\alpha]_D$ -63.9 (c, 0.36 in $CHCl_3$).

Gandolfi, C. *et al., Tet. Lett.*, 1970, **11**, 1677-1680 (*synth*)
Cambiaghi, S. *et al., Ann. Chim. (Rome)*, 1971, **61**, 99; *CA*, **75**, 36397x (*Isojuripidine*)
Chakravarty, A.K. *et al., Phytochemistry*, 1983, **22**, 2843-2845 (*Juripidine*)
Silva, T.M.S. *et al., J. Braz. Chem. Soc.*, 2005, **16**, 1467-1471 (*Isojuripidine*)

3-Aminospirostan-9-ol, 9CI A-910



$C_{27}H_{45}NO_3$ 431.657

(3β,5α,25R)-form
Isopaniculidine
[16577-35-8]
Alkaloid from *Solanum paniculatum* (Solanaceae). Mp 202-204°. $[\alpha]_D$ -70 (c, 0.01 in $CHCl_3$).

N-*Ac:* Mp 282-284°.

(3β,5α,25S)-form
Paniculidine
[16577-34-7]
Alkaloid from *Solanum paniculatum* (Solanaceae). Needles (MeOH). Mp 228-244°. $[\alpha]_D^{22}$ -82.2 (c, 1.447 in $CHCl_3$).

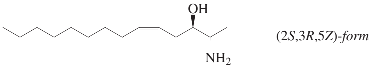
Cambiaghi, S. *et al., Ann. Chim. (Rome)*, 1971, **61**, 99; *CA*, **75**, 36397x (*ir, pmr, isol, struct*)

14-Aminotetradecanoic acid A-911

14-Aminomyristic acid
[17437-20-6]
$H_2NCH_2(CH_2)_{12}COOH$
$C_{14}H_{29}NO_2$ 243.389
Constit. of the roots of *Decalepis hamiltonii*. Antioxidant. Mp 178-179°.

Hünig, S. *et al., Chem. Ber.*, 1967, **100**, 3039-3044 (*synth*)
Srivastava, A. *et al., J. Agric. Food Chem.*, 2006, **54**, 790-795 (*isol, pmr, cmr*)

2-Amino-5-tetradecen-3-ol A-912



$C_{14}H_{29}NO$ 227.389

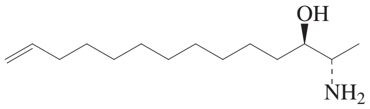
(2S,3R,5Z)-form
Halaminol C
[389125-68-2]
Isol. from a marine sponge *Haliclona* n. sp. Oil. $[\alpha]_D$ +1.9 (c, 0.025 in CH_2Cl_2).

(2S,3S,5E)-form [181523-19-3]

N,O-*Di-Ac:* [181523-11-5]
$C_{18}H_{33}NO_3$ 311.464
Isol. from a marine ascidian (*Pseudodistoma* sp.).

Hooper, G.J. *et al., Nat. Prod. Lett.*, 1995, **6**, 31-35 (*isol*)
Clark, R.J. *et al., J. Nat. Prod.*, 2001, **64**, 1568-1571 (*isol, pmr, cmr*)
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*abs config*)

2-Amino-13-tetradecen-3-ol A-913



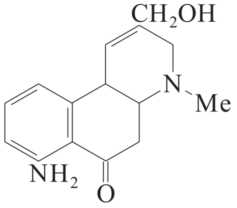
$C_{14}H_{29}NO$ 227.389

(2S,3R)-form
Halaminol A
[389125-56-8]
Isol. from the marine sponge *Haliclona* n. sp. Oil. $[\alpha]_D$ +1.7 (c, 0.04 in CH_2Cl_2). $[\alpha]_D$ -30 (c, 0.003 in MeOH) (as *N,O*-di-Ac).

Clark, R.J. *et al., J. Nat. Prod.*, 2001, **64**, 1568-1571 (*Halaminol A, isol, pmr, cmr*)

7-Amino-3,4,4*a*,10*b*-tetrahydro-2-(hydroxymethyl)-4-methylbenzo[*f*]quinolin-6(5*H*)-one A-914

[134677-39-7]



$C_{15}H_{18}N_2O_2$ 258.319
Isol. from *Claviceps purpurea*. Cryst. (Et_2O). Prob. a degradn. prod. of ergot alkaloids.

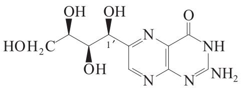
Deoxy: ***7-Amino-3,4,4a,10b-tetrahydro-2,4-dimethylbenzo[f]quinolin-6(5H)-one***
[134677-38-6]

$C_{15}H_{18}N_2O$ 242.32
Isol. from *Claviceps purpurea*. Cryst. (Me_2CO). Prob. a degradn. prod. of ergot alkaloids.

Flieger, M. *et al., J. Nat. Prod.*, 1991, **54**, 390 (*isol, pmr, cmr, ms, struct*)

2-Amino-6-(1,2,3,4-tetrahydroxybutyl)-4(1*H*)-pteridinone, 9CI A-915

2-Amino-4-hydroxy-6-(1,2,3,4-tetrahydroxybutyl)pteridine. Rs I
[13392-23-9]



(1′*R*,2′*S*,3′*R*)–*form*

$C_{10}H_{13}N_5O_5$ 283.243

(1′*R*,2′*S*,3′*R*)-*form*
ᴅ-arabino-*form*
[735-67-1]
$[\alpha]_D$ -97.3 (c, 0.3 in 0.1*M* NaOH). Dec. slowly above 220°.

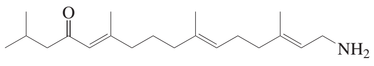
(1′*R*,2′*S*,3′*S*)-*form*
ʟ-xylo-*form*
[153829-74-4]
$[\alpha]_D$ -69 (c, 0.4 in 0.1*M* NaOH).

(1′*S*,2′*S*,3′*R*)-*form*
ᴅ-ribo-*form*
[153829-70-0]
Isol. from *Rhodopseudomonas spheroides*.

[735-67-1 , 95840-18-9 , 153829-73-3 , 153829-71-1 , 153829-72-2 , 95191-28-9]

Petering, H.G. *et al., J.A.C.S.*, 1949, **71**, 3977 (*synth*)
Henseke, G. *et al., Chem. Ber.*, 1956, **89**, 2904 (*synth*)
Taylor, E.C. *et al., J.A.C.S.*, 1976, **98**, 2301 (*synth*)
Seo, N. *et al., Biochim. Biophys. Acta*, 1991, **1074**, 439 (*isol*)
Hariu, T. *et al., Pteridines*, 1993, **4**, 63 (*abs config*)

16-Amino-2,6,10,14-tetramethyl-5,10,14-hexadecatrien-4-one A-916



(5*E*,10*E*,14*E*)-*form*

$C_{20}H_{35}NO$ 305.503

(5*E*,10*E*,14*E*)-*form*
N-*Formyl:* ***Malonganenone H***
[945458-51-5]
$C_{21}H_{35}NO_2$ 333.513
Isol. from *Euplexaura nuttingi*. Oil.

(5*Z*,10*E*,14*E*)-*form*
N-*Formyl:* ***Malonganenone C***
[882403-71-6]
$C_{21}H_{35}NO_2$ 333.513
Isol. from *Leptogorgia gilchristi*. Yellow solid. λ_{max} 230 (ε 8800); 276 (ε 1400) (MeOH).

Keyzers, R.A. *et al., Tetrahedron*, 2006, **62**, 2200-2206 (*Malonganenone C*)
Sorek, H. *et al., J. Nat. Prod.*, 2007, **70**, 1104-1109 (*Malonganenone H*)

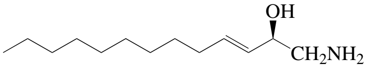
1-Amino-4,12-tridecadien-2-ol, 9CI A-917

$H_2C{=}CH(CH_2)_6CH{=}$
$CHCH_2CH(OH)CH_2NH_2$
$C_{13}H_{25}NO$ 211.347

(±)-(*E*)-*form* [181523-21-7]
N,O-*Di-Ac:* [181523-13-7]
$C_{17}H_{29}NO_3$ 295.421
Isol. from a marine ascidian (*Pseudodistoma* sp.).

Hooper, G.J. *et al., Nat. Prod. Lett.*, 1995, **6**, 31-35 (*isol*)

1-Amino-3-tridecen-2-ol A-918



$C_{13}H_{27}NO$ 213.362

(2*R*,3*E*)-*form* [150922-61-5]
Isol. from the ascidian *Didemnum* sp.

Searle, P.A. *et al., J.O.C.*, 1993, **58**, 7578-7580 (*isol*)

1-Amino-5-tridecen-2-ol A-919

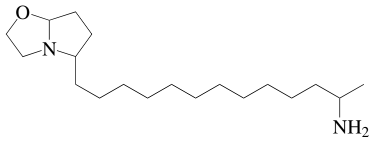
$C_{13}H_{27}NO$ 213.362

(2*R*,5*E*)-*form* [150922-60-4]
Isol. from the ascidian *Didemnum* sp. Antifungal agent. $[\alpha]_D$ +1.9 (c, 0.4 in MeOH) (as trifluoroacetate salt).

Searle, P.A. *et al., J.O.C.*, 1993, **58**, 7578-7580 (*isol, ir, pmr, abs config*)

5-(12-Aminotridecyl)hexahydropyrrolo[2,1-*b*]oxazole A-920

*Hexahydro-α-methylpyrrolo[2,1-*b*]oxazole-5-dodecanamine, 9CI*
[192213-01-7]

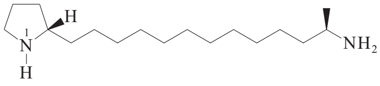


$C_{19}H_{38}N_2O$ 310.522
Alkaloid from the ladybirds *Epilachna boraelis* and *Epilachna varivestis.*

Radford, P. *et al., J. Nat. Prod.*, 1997, **60**, 755-759 (*isol, pmr, cmr, ms*)

2-(12-Aminotridecyl)pyrrolidine A-921

α-Methyl-2-pyrrolidinedodecanamine, 9CI. 13-(2-Pyrrolidinyl)-2-tridecylamine



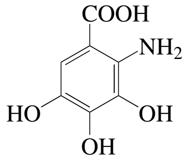
$C_{17}H_{36}N_2$ 268.485

(2*S*,12′*R*)-*form* [151751-64-3]
Alkaloid from whole body extracts of the Mexican bean beetle *Epilachna varivestis.* $[\alpha]_D^{22}$ +9.3 (c, 0.15 in $CDCl_3$).
N^1-*(2-Hydroxyethyl): 2-(12-Aminotridecyl)-1-pyrrolidineethanol, 9CI.* ***1-(2-Hydroxyethyl)-2-(12-aminotridecyl)-pyrrolidine***
[151751-65-4]
$C_{19}H_{40}N_2O$ 312.538
Alkaloid present in eggs, larvae, pupae and adults of *Epilachna varivestis.* $[\alpha]_D^{22}$ +38.8 (c, 0.18 in $CDCl_3$).

Attygalle, A.B. *et al., Tetrahedron*, 1993, **49**, 9333 (*isol, ir, pmr, cmr, ms, struct*)
Shi, X. *et al., Tetrahedron*, 1996, **52**, 6859 (*isol, pmr, cmr, ms, synth, abs config*)
Shi, X. *et al., Tet. Lett.*, 1997, **38**, 6479 (*synth, abs config*)

2-Amino-3,4,5-trihydroxybenzoic acid, 9CI A-922

3,4,5-Trihydroxyanthranilic acid, 9CI



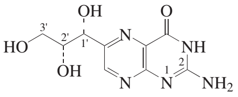
$C_7H_7NO_5$ 185.136

5-Me ether: 2-Amino-3,4-dihydroxy-5-methoxybenzoic acid
[1035536-86-7]
$C_8H_9NO_5$ 199.163
Alkaloid from the leaves of *Cyclocarya paliurus.* Needles. Mp 186-188°. λ_{max} 290 (ε 3450) ($CHCl_3$).
Tri-Me ether: 2-Amino-3,4,5-trimethoxybenzoic acid
[61948-85-4]
$C_{10}H_{13}NO_5$ 227.216
Mp 138-140°.
Tri-Me ether, Me ester: [5035-82-5]
$C_{11}H_{15}NO_5$ 241.243
Mp 44-45°. $Bp_{0.1}$ 127-140°.

Hammen, P.D. *et al., J. Het. Chem.*, 1987, **24**, 1701-1704
Li, J. *et al., Planta Med.*, 2008, **74**, 287-289 (*5-Me ether, isol*)

2-Amino-6-(1,2,3-trihydroxypropyl)-4(1*H*)-pteridinone, 9CI A-923

[670-65-5]



(1'*R*,2'*R*)-*form*

$C_9H_{11}N_5O_4$ 253.217

(1′*R*,2′*R*)-*form*
ᴅ-threo-*form*. ***ᴅ-Monapterin***. *Umanopterin*
[10162-32-0]
Isol. from *Tetrahymena pyriformis* and from the urine of cancer patients. $[\alpha]_D^{25}$ -92 (c, 0.3 in 0.1*M* HCl).
*5,6*R*,7,8-Tetrahydro:* ***5,6,7,8-Tetrahydro-ᴅ-monapterin***
[99630-31-6]

$C_9H_{15}N_5O_4$ 257.249
Isol. from *Tetrahymena pyriformis.*

(1′S,2′S)-form
L-threo-*form.* ***L-Monapterin***
[2277-42-1]
Constit. of human blood and urine. Yellow cryst. $[\alpha]_D^{25}$ +97 (c, 0.3 in 0.1*M* HCl).

*2-*N,N*-Di-Me: 2-Dimethylamino-6-(1,2,3-trihydroxypropyl)-4(3*H*)-pteridinone.* ***Euglenapterin***
[73789-39-6]
[73789-45-4]
$C_{11}H_{15}N_5O_4$ 281.271
Found in the alga *Euglena gracilis.* Yellow cryst. (H_2O). Mp 200°. Yellow fluor. in soln.

*2-*N,N*-Di-Me, 3′-phosphate:*
$C_{11}H_{16}N_5O_7P$ 361.251
Found in the alga *Euglena gracilis.* Yellow fluor. in soln.

*2-*N,N*-Di-Me, 2′,3′-cyclic phosphate:*
$C_{11}H_{14}N_5O_6P$ 343.235
Found in the alga *Euglena gracilis.* Yellow fluor. in soln.

*5,6*R*,7,8-Tetrahydro:* ***5,6,7,8-Tetrahydro-L-monapterin***
[348622-74-2]
$C_9H_{15}N_5O_4$ 257.249
Isol. from *Escherichia coli.* Needles ($CHCl_3$) (as hexa-Ac). Mp 139.5-141.5° (hexa-Ac).

(1′S,2′R)-form
D-erythro-*form.* ***Neopterin***
[2009-64-5]
Found in human blood and urine. First isol. from the pupae of bees. Precursor in biosynth. of 2-Amino-6-(1,2-dihydroxypropyl)-4(1*H*)-pteridinone, A-749. $[\alpha]_D^{25}$ +45 (c, 0.3 in 0.1*M* HCl).

*3′-*O*-β-D-Glucopyranoside:* ***Solfapterin****. Neopterin 3-*O*-β-D-glucoside*
[114312-02-6]
$C_{15}H_{21}N_5O_9$ 415.359
Isol. from *Sulfolobus solfataricus.*

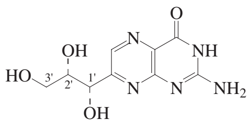
(1′R,2′S)-form
L-erythro-*form.* ***Bufochrome***
[2277-43-2]
Found in human blood and urine. Also isol. from toad skins. Growth factor for the protozoan *Crithidia fasiculata*. $[\alpha]_D^{25}$ -44 (c, 0.3 in 0.1*M* HCl). λ_{max} 275 (ε 14600); 348 (ε 6180) (H_2O). λ_{max} 255 (ε 24000); 365 (ε 7050) (0.1*M* NaOH). λ_{max} 248 (ε 11600); 321 (ε 8020) (0.1*M* HCl).

[39923-31-4 , 87174-05-8 , 81873-20-3]

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 480C (*nmr*)
Rembold, H. *et al., Chem. Ber.*, 1963, **96**, 1406 (*struct, synth*)
Andrews, K.J.M. *et al., Chem. Comm.*, 1968, 120
v. Viscontini, M. *et al., Helv. Chim. Acta*, 1968, **51**, 1495 (*synth, pmr*)
Fukushima, T. *et al., J. Biol. Chem.*, 1972, **247**, 4549 (*isol*)
Elstner, E. *et al., Arch. Biochem. Biophys.*, 1976, **173**, 614 (*Euglenapterin*)
Schircks, B. *et al., Helv. Chim. Acta*, 1976, **59**, 248 (*cmr*)
Sugimoto, T. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 2344 (*synth*)
Fukushima, T. *et al., Methods Enzymol.*, 1980, **66**, 508 (*rev, isol*)
Jacobi, P.A. *et al., J.O.C.*, 1981, **46**, 5416 (*Euglenapterin, synth*)
Sun, J.H. *et al., Diss. Abstr. Int., B*, 1983, **43**, 3990 (*synth*)
Böhme, M. *et al., Annalen*, 1986, 1705 (*Euglenapterin, isol, cryst struct, uv, cd, pmr, synth*)
Zeitler, H.J. *et al., Methods Enzymol.*, 1986, **122**, 273 (*rev, detn*)
Huber, C. *et al., Dtsch. Med. Wochenschr.*, 1987, **112**, 107 (*rev*)
Lin, X. *et al., J. Bacteriol.*, 1988, **170**, 1396 (*Solfapterin*)
Klein, R. *et al., Biochimie*, 1991, **73**, 1281 (*D-Monapterin*)
Ogiwara, S. *et al., Biol. Chem. Hoppe-Seyler*, 1992, **373**, 1061 (*isol*)
Ogiwara, S. *et al., Tet. Lett.*, 1992, **33**, 1341 (*Umanopterin*)
Sugimoto, T. *et al., Helv. Chim. Acta*, 2001, **84**, 918-927 (*Tetrahydro-D-monapterin*)
Ikemoto, K. *et al., Biol. Chem.*, 2002, **383**, 325-330 (*Tetrahydro-L-monapterin*)
Chen, N. *et al., Heterocycles*, 2005, **65**, 2917-2924 (*acetates, cd, abs config*)

2-Amino-7-(1,2,3-trihydroxypropyl)-4(1*H*)-pteridinone A-924

7-(1,2,3-Trihydroxypropyl)pterin



(1′*R*,2′*S*)-*form*

$C_9H_{11}N_5O_4$ 253.217
Abnormal pterin isol. from urine of patients with atypical phenylketonuria (abs. config. of nat. metab. not yet known).

(1′R,2′S)-form
L-erythro-*form*
$[\alpha]_D$ -13.

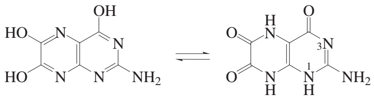
3′-Deoxy: ***Primapterin****. 7-Biopterin*
[2636-52-4]
$C_9H_{11}N_5O_3$ 237.218
Occurs in urine of patients with atypical phenylketonuria. Also in patients with hyperphenylalaninemia. $[\alpha]_D^{22}$ -37.4 (c, 0.1 in 0.1*M* HCl).

(1′S,2′R)-form
D-erythro-*form.* ***Anapterin****. 7-Neopterin*
[126779-19-9]
Occurs in urine of patients with hyperphenylalaninemia. Microcryst. (H_2O). $[\alpha]_D^{22}$ +19.5 (c, 0.4 in 1*M* HCl). CA erroneously names Anapterin as 7-(12-dihydroxypropyl)pterin.

Rembold, H. *et al., Chem. Ber.*, 1963, **96**, 1395-1405 (*7-Biopterin, synth, uv*)
Curtis, H.-C. *et al., Biochem. Biophys. Res. Commun.*, 1988, **153**, 715-721 (*Anapterin, Primapterin, isol*)
Viscontini, M. *et al., Helv. Chim. Acta*, 1990, **73**, 337-345 (*Primapterin, Anapterin, synth, cd, pmr, bibl*)
Curtius, H.-C. *et al., J. Biol. Chem.*, 1990, **265**, 3923-3930 (*7-Neopterin, 7-Biopterin, isol*)

2-Amino-4,6,7-trihydroxypteridine A-925

*2-Amino-5,8-dihydro-4,6,7(1*H*)-pteridinetrione, 9CI.* ***Leucopterin***
[492-11-5]



$C_6H_5N_5O_3$ 195.137
Found in the wings of many butterflies, e.g. *Pieris brassicae*. Cryst. Blue fluor. in alkaline soln. Forms yellow salts.

Wieland, Th. *et al., Annalen*, 1940, **544**, 172 (*synth*)
Pfleiderer, W. *et al., Chem. Ber.*, 1957, **90**, 2631; 1961, **94**, 118 (*synth, struct*)
Mueller, G. *et al., Helv. Chim. Acta*, 1973, **56**, 2680 (*cmr*)
Pfleiderer, W. *et al., J. Het. Chem.*, 1992, **29**, 583 (*rev*)

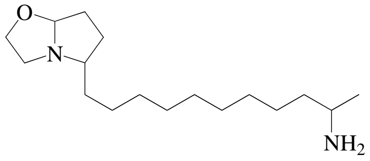
4-Amino-*N,N,N*-tris(3-aminopropyl)-1-butanaminium, 9CI A-926

N^4,N^4-Bis(3-aminopropyl)spermidine
[143085-76-1]
$(H_2NCH_2CH_2CH_2)_3N^+(CH_2)_3CH_2NH_2$
$C_{13}H_{34}N_5^{\oplus}$ 260.445
Isol. from the thermophilic bacteria *Bacillus schlegelii, Thermoleophilum album, Thermoleophilum minutum, Hydrogenobacter thermophilus* and *Hydrogenobacter halophilus.* Counterion not specified.

Hamana, K. *et al., Biochem. J.*, 1992, **284**, 741-747 (*isol*)

5-(10-Aminoundecyl)hexahydropyrrolo[2,1-*b*]oxazole A-927

*Hexahydro-α-methylpyrrolo[2,1-*b*]oxazole-5-decanamine, 9CI*
[192213-02-8]

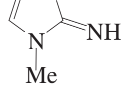


$C_{17}H_{34}N_2O$ 282.468
Alkaloid from the ladybird *Epilachna borealis.*

Radford, P. *et al., J. Nat. Prod.*, 1997, **60**, 755-759 (*isol, ms*)

Aminozooanemonin A-928

*2,3-Dihydro-2-imino-1,3-dimethyl-1*H*-imidazole-4-acetic acid, 9CI*
[213749-79-2]



$C_7H_{11}N_3O_2$ 169.183

Prototropic guanidino system showing zwitterion formation. Shown here and in the CAS name as the neutral species. Alkaloid from the sponge *Agelas dispar*. Amorph. solid. λ_{max} 226 (ϵ 3500); 262 (ϵ 1500) (MeOH).

Cafieri, F. *et al., J. Nat. Prod.*, 1998, **61**, 1171-1173 (*isol, uv, ir, pmr, cmr*)

Ammocalline A-929

[1354-30-9]

$C_{19}H_{22}N_2$ 278.396

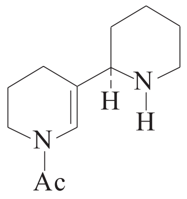
Struct. unknown. Alkaloid from roots of *Catharanthus roseus* (Apocynaceae). Needles (Me_2CO). Mp 335° dec. pK_a 7.3 (33% DMF aq.).

Svoboda, G.H. *et al., J. Nat. Prod.*, 1963, **26**, 141-153 (*isol, ir, uv*)

Ammodendrine A-930

1-Acetyl-1,2,3,4-tetrahydro-5-(2-piperidinyl)pyridine, 9CI. 1′-Acetyl-1,1′,2,3,4,4′,5,5′,6,6′-decahydro-2,3′-bipyridine. N-*Acetyl-*Δ^2*-tetrahydroanabasine. Sphaerocarpine*

[27542-15-0]



$C_{12}H_{20}N_2O$ 208.303

▶ Exp. teratogen.

***(R)*-form**

Isoammodendrine

[494-15-5]

Alkaloid from *Genista sphaerocarpa, Ammodendron conollyi, Lupinus formosus* and other plant spp. Cryst. or oil. Mp 43-46°. $[\alpha]_D^{24}$ +5.4 (c, 1.3 in MeOH). Many isolates with higher opt rotations were probably contaminated.

▶ UR9150000

Perchlorate:

Cryst. (H_2O or Me_2CO). Mp 210-211°.

N-*Formyl:* **N′-*Formylammodendrine***

[53508-17-1]

$C_{13}H_{20}N_2O_2$ 236.313

Alkaloid from *Dichilus strictus* and *Spartidium saharae.*

N-*Me:* **N′-*Methylammodendrine***

[52196-10-8]

$C_{13}H_{22}N_2O$ 222.33

Alkaloid in *Lupinus formosus* (Fabaceae). Oil (natural), cryst. (petrol)(-synthetic). Mp 65-66°. $[\alpha]_D^{23}$ +62.4 (c, 0.5 in MeOH).

(±)-*form* [20824-32-2]

Alkaloid from *Ammodendron conollyi*, other *Ammodendron* spp. *Sophora franchetiana* and *Coelidium fourcadei* (Fabaceae). Mp 50-60°.

Monohydrate: Mp 73-74°.

Hydroiodide:

Cryst. (EtOH). Mp 221-222°.

N-*Me:*

Cryst. (petrol). Mp 65-66°.

N-*Me; hydroiodide:* Mp 184-185°.

(ξ)-*form*

Alkaloid from *Ammodendron karelinii, Ammodendron longiracemosum, Ammodendron lehmanni, Genista hystrix, Lupinus mutabilis, Castilleja miniata, Ammopiptanthus mongolicus, Thermopsis lupinoides* and other plants (opt. rotn. of these isolates mostly unreported) (Fabaceae).

Orekhov, A.P. *et al., Ber.*, 1935, **68**, 1807 (*isol*)
Orekhov, A.P. *et al., Bull. Soc. Chim. Fr.*, 1938, **5**, 29 (*struct*)
Dominguez, J. *et al., An. R. Soc. Esp. Fis. Quim., Ser. B*, 1956, 43; *CA*, **51**, 1212h (*struct, resoln*)
Ribas-Marques, I. *et al., An. R. Soc. Esp. Fis. Quim., Ser. B*, 1962, **57**, 781; *CA*, **58**, 5738c (*abs config*)
Schöpf, C. *et al., Annalen*, 1964, **674**, 87 (*synth*)
Arndt, R.R. *et al., J. S. Afr. Chem. Inst.*, 1968, **21**, 54; *CA*, **70**, 4342f (*isol, pmr*)
Fitch, W.L. *et al., J.A.C.S.*, 1974, **96**, 4917 (*ms*)
Fitch, W.L. *et al., J.O.C.*, 1974, **39**, 2974 (*isol, deriv*)
Kushmuradov, Yu.K. *et al., Khim. Prir. Soedin.*, 1977, 717; 1979, 871; *Chem. Nat. Compd. (Engl. Transl.)*, 604; 780 (*isol*)
Tashkhodzhaev, B. *et al., Khim. Prir. Soedin.*, 1982, 661; *Chem. Nat. Compd. (Engl. Transl.)*, 631 (*cryst struct*)
Van Wyk, B.E. *et al., S. Afr. J. Bot.*, 1989, **55**, 523 (*N′-Formylammodendrine*)
Lee, S.T. *et al., J. Nat. Prod.*, 2005, **68**, 681-685 (*isol, resoln, tox*)

Ammorosine A-931

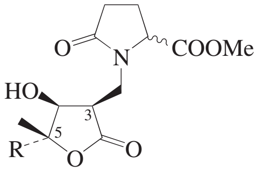
[1354-31-0]

Struct. unknown. Alkaloid from roots of *Catharanthus roseus* (Apocynaceae). Blades (MeOH). Mp 221-225°. pK_a 7.3 (33% DMF aq.).

Svoboda, G.H. *et al., J. Nat. Prod.*, 1963, **26**, 141-153 (*isol, ir, uv*)

Amphiasterin C_1 A-932

[330680-37-0]



$R = -(CH_2)_3\overset{4''}{C}H{=}\overset{5''}{C}H(CH_2)_9CH_3(E\text{-})$

Relative Configuration

$C_{27}H_{45}NO_6$ 479.656

Isol. from *Plakortis quasiamphiaster*. Oil. $[\alpha]_D^{20}$ -19.3 (c, 0.14 in $CHCl_3$).

4″,5″-Dihydro: ***Amphiasterin*** C_3

[330680-39-2]

$C_{27}H_{47}NO_6$ 481.671

Isol. from *Plakortis quasiamphiaster*. Oil. $[\alpha]_D^{20}$ -8 (c, 0.4 in $CHCl_3$).

3-Epimer: ***Amphiasterin*** D_1

[330680-41-6]

$C_{27}H_{45}NO_6$ 479.656

Isol. from *Plakortis quasiamphiaster*. Oil. $[\alpha]_D^{20}$ -16 (c, 0.06 in $CHCl_3$).

3,4,5-Triepimer: ***Amphiasterin*** E_1

[330680-44-9]

$C_{27}H_{45}NO_6$ 479.656

Isol. from *Plakortis quasiamphiaster*. Oil. $[\alpha]_D^{20}$ -3.8 (c, 0.11 in $CHCl_3$).

Zampella, A. *et al., Tetrahedron*, 2001, **57**, 257-263 (*Amphiasterins* C_1,C_3,D_1,E_1)

Amphiasterin C_2 A-933

[330680-38-1]

As Amphiasterin C_1, A-932 with

$R = -(CH_2)_5CH{=}CH(CH_2)_9CH_3(E\text{-})$

$C_{29}H_{49}NO_6$ 507.709

Isol. from *Plakortis quasiamphiaster*. Oil. $[\alpha]_D^{20}$ -12.3 (c, 0.65 in $CHCl_3$).

6″,7″-Dihydro: ***Amphiasterin*** C_4

[330680-40-5]

$C_{29}H_{51}NO_6$ 509.725

Isol. from *Plakortis quasiamphiaster*. Oil. $[\alpha]_D^{20}$ -11.5 (c, 0.13 in $CHCl_3$).

3-Epimer: ***Amphiasterin*** D_2

[330680-42-7]

$C_{29}H_{49}NO_6$ 507.709

Isol. from *Plakortis quasiamphiaster*. Oil. $[\alpha]_D^{20}$ -2.9 (c, 0.24 in $CHCl_3$).

3-Epimer, 6″,7″-dihydro: ***Amphiasterin*** D_3

[330680-43-8]

$C_{29}H_{51}NO_6$ 509.725

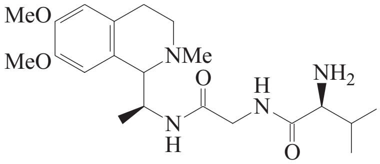
Isol. from *Plakortis quasiamphiaster*. Oil. $[\alpha]_D^{20}$ -1.5 (c, 0.1 in $CHCl_3$).

Zampella, A. *et al., Tetrahedron*, 2001, **57**, 257-263 (*Amphiasterins* C_2,C_4,D_2,D_3)

Amphibine I A-934

*L-Valyl-*N*-[1-(1,2,3,4-tetrahydro-6,7-dimethoxy-2-methyl-1-isoquinolinyl)ethyl]-glycinamide, 9CI*

[53098-67-2]



$C_{21}H_{34}N_4O_4$ 406.524

Consists of mixt. of diastereoisomer shown with 1,9-diepimer. Alkaloid from *Zizyphus amphibia* (Rhamnaceae). Pale yellow foam. $[\alpha]_D^{20}$ -50 (c, 0.6 in C_6H_6).

Hydrochloride (1:2):

Cryst. ($CHCl_3$/petrol). Mp 175° dec. $[\alpha]_D^{20}$ -3.4 (c, 0.24 in MeOH).

N-*Ac:*

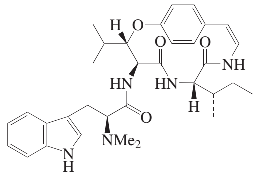
Needles (CH_2Cl_2). Mp 188-190°. $[\alpha]_D^{20}$ -20 (c, 0.1 in EtOH).

Tschesche, R. *et al., Chem. Ber.*, 1974, **107**, 1329; 1975, **108**, 2247 (*ir, uv, ms, pmr, isol, struct, synth, config, cd*)

Koyama, J. *et al., Heterocycles*, 1978, **9**, 443 (*synth, cd*)

Amphibine A A-935

[36535-97-4]



Absolute Configuration

$C_{33}H_{43}N_5O_4$ 573.734

Prob. identical with Discarine A and possibly also with Waltherine B. Alkaloid from the bark of *Zizyphus amphibia* and *Zizyphus spinachristi* and from the root bark of *Zizyphus nummularia* (Rhamnaceae). Needles (CH_2Cl_2/MeOH). Mp 237-239° dec. $[\alpha]_D^{20}$ -310 (c, 0.021 in MeOH).

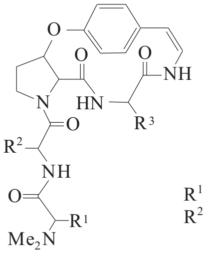
Stereoisomer (1)(?): ***Waltherine B***
[243464-60-0]
$C_{33}H_{43}N_5O_4$ 573.734
Alkaloid from the root bark of *Waltheria douradinha*. Needles ($CHCl_3$/MeOH). Mp 242-243°. $[\alpha]_D^{20}$ -201.8 (c. 0.21 in MeOH).

Stereoisomer (2)(?): ***Discarine A***
[36211-12-8]
$C_{33}H_{43}N_5O_4$ 573.734
Alkaloid from the roots of *Discaria longispina* (Rhamnaceae). Cryst. (CH_2Cl_2/Et_2O). Mp 229-231°. $[\alpha]_D$ -282 (c, ca. 0.05 in $CHCl_3$).

González Sierra, M. *et al., Chem. Comm.*, 1972, 915-916 (*Discarine A, pmr, stereochem*)
Mascaretti, O.A. *et al., Phytochemistry*, 1972, **11**, 1133 (*Discarine A, isol, struct*)
Tschesche, R. *et al., Tet. Lett.*, 1972, 865-868 (*Amphibine A, ms, struct*)
Tschesche, R. *et al., Phytochemistry*, 1974, **13**, 1633 (*Amphibine A, isol*)
Tschesche, R. *et al., Tetrahedron*, 1975, **31**, 2944-2947 (*Amphibine A, isol*)
Païs, M. *et al., Phytochemistry*, 1979, **18**, 1869-1872 (*Discarine A, cmr*)
Morel, A.F. *et al., Phytochemistry*, 1999, **51**, 473-477 (*Waltherine B, isol*)

Amphibine B A-936

[38541-74-1]



$R^1 = R^3 = CH_2Ph$
$R^2 = CH(CH_3)CH_2CH_3$

$C_{39}H_{47}N_5O_5$ 665.831

Stereochem. not yet determined. Alkaloid from the bark of *Zizyphus amphibia* and *Zizyphus rugosa*, and from *Ziziphus oenoplia*, *Zizyphus mauritiana* (Rhamnaceae). Amorph. $[\alpha]_D^{20}$ -181 (c, 0.08 in MeOH). λ_{max} 210 (end) ; 260 (sh) (MeOH).

Tschesche, R. *et al., Chem. Ber.*, 1972, **105**, 3094-3105 (*Zizyphus amphibia constit, struct*)
Tschesche, R. *et al., Annalen*, 1974, 1694-1701 (*Ziziphus mauritiana constit*)
Singh, A. *et al., J. Indian Chem. Soc.*, 2008, **85**, 658-659 (*Zizyphus rugosa constit*)

Amphibine C A-937

[38496-01-4]

As Amphibine B, A-936 with
$R^1 = CH_2CH(CH_3)_2$, $R^2 = CH(CH_3)CH_2CH_3$, $R^3 = CH_2Ph$

$C_{36}H_{49}N_5O_5$ 631.814

Alkaloid from the bark of *Zizyphus amphibia* (Rhamnaceae). Amorph. $[\alpha]_D^{20}$ -224 (c, 0.075 in MeOH).

Tschesche, R. *et al., Chem. Ber.*, 1972, **105**, 3094 (*isol, uv, cd, ir, pmr, ms, struct*)

Amphibine D A-938

[38496-02-5]

As Amphibine B, A-936 with
$R^1 = CH_2Ph$, $R^2 = R^3 = CH(CH_3)CH_2CH_3$

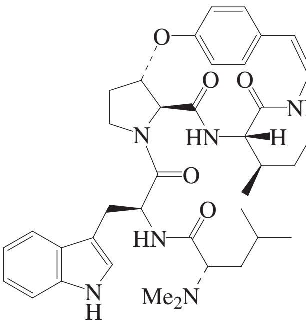
$C_{36}H_{49}N_5O_5$ 631.814

Alkaloid from the bark of *Zizyphus amphibia*, *Zizyphus mauritiana*, *Zizyphus rugosa* and *Zizyphus juazeiro* (Rhamnaceae). Amorph. $[\alpha]_D^{20}$ -203 (c, 0.09 in MeOH).

Tschesche, R. *et al., Chem. Ber.*, 1972, **105**, 3094-3105 (*isol, uv, cd, ir, pmr, ms, struct*)
Hindenlang, D.M. *et al., Annalen*, 1980, 447-450 (*cmr*)
Tschesche, R. *et al., Pharmazie*, 1981, **36**, 511 (*isol, uv, ir, pmr, ms*)

Amphibine E A-939

[38541-75-2]



$C_{38}H_{50}N_6O_5$ 670.85

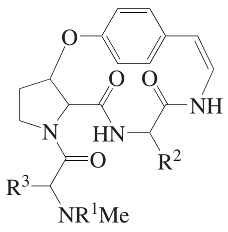
Alkaloid from the bark of *Zizyphus amphibia*, *Zizyphus mauritiana* and *Zizyphus spinachristi* (Rhamnaceae). Amorph. $[\alpha]_D^{20}$ -175 (c, 0.14 in MeOH).

N-*De-Me:* ***Mauritine J***
[177715-71-8]
$C_{37}H_{48}N_6O_5$ 656.823
Alkaloid from root bark of *Zizyphus mauritiana*. Amorph. $[\alpha]_D$ -175.9 (c, 1.0 in MeOH).

Tschesche, R. *et al., Chem. Ber.*, 1972, **105**, 3094-3105 (*isol, uv, cd, ir, pmr, ms, struct*)
Tschesche, R. *et al., Annalen*, 1974, 1694-1702 (*isol*)
Tschesche, R. *et al., Phytochemistry*, 1974, **13**, 1633 (*isol*)
Hindenlang, D.M. *et al., Annalen*, 1980, 447-450 (*cmr*)
Jossang, A. *et al., Phytochemistry*, 1996, **42**, 565-567 (*Mauritine J*)

Amphibine F A-940

[52617-26-2]



$R^1 = H$, $R^2 = -CH_2Ph$
$R^3 = -CH(CH_3)CH_2CH_3$

$C_{29}H_{36}N_4O_4$ 504.628

Alkaloid from the bark of *Zizyphus amphibia*, *Zizyphus mauritiana* and *Zizyphus spinachristi* (Rhamnaceae). Amorph. $[\alpha]_D^{20}$ -171 (c, 0.26 in $CHCl_3$).

Dihydro, N-*Me:*
Needles (Me_2CO/cyclohexane). Mp 152-156°. $[\alpha]_D^{20}$ -119 (c, 0.05 in $CHCl_3$).

Tschesche, R. *et al., Chem. Ber.*, 1974, **107**, 686 (*isol, uv, ir, pmr, ms, struct*)
Tschesche, R. *et al., Annalen*, 1974, 1694 (*isol*)
Tschesche, R. *et al., Phytochemistry*, 1974, **13**, 1633 (*isol*)

Amphibine G A-941

[52617-27-3]

As Amphibine F, A-940 with
$R^1 = Me$, $R^2 = –CH_2CH(CH_3)_2$, $R^3 =$ 3-Indolyl–CH_2–

$C_{32}H_{39}N_5O_4$ 557.691

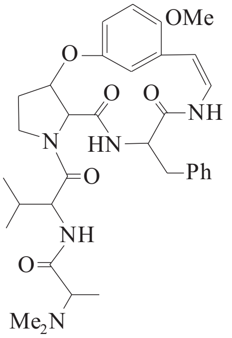
Alkaloid from the bark of *Zizyphus amphibia* (Rhamnaceae). Needles (CCl_4). Mp 182-185°. $[\alpha]_D^{20}$ -218 (c, 0.24 in $CHCl_3$).

Dihydro:
Amorph. $[\alpha]_D^{20}$ +119 (c, 0.2 in $CHCl_3$).

Tschesche, R. *et al., Chem. Ber.*, 1974, **107**, 686 (*isol, uv, cd, ir, pmr, ms, struct*)

Amphibine H A-942

[52659-55-9]



$C_{33}H_{43}N_5O_6$ 605.733

Alkaloid from the bark or root bark of *Zizyphus amphibia*, *Zizyphus nummularia*, *Zizyphus jujuba*, *Zizyphus spina-christi* and *Zizyphus xylopyra*. Shows antibacterial activity. Cryst. ($CHCl_3$/petrol). Mp 205°. $[\alpha]_D^{20}$ -570 (c, 0.12 in MeOH).

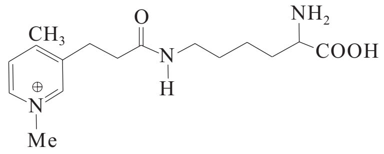
N-*De-Me:* ***Nummularine B***. N-*Demethylamphibine H. Daechuine S27*
[53947-96-9]
$C_{32}H_{41}N_5O_6$ 591.706
Alkaloid from the root bark or stem bark of *Zizyphus nummularia*, *Zizyphus jujuba*, *Zizyphus sativa* and *Zizyphus xylopyra* (Rhamnaceae). Shows antibacterial activity. Needles (MeOH). Mp 230-231°. $[\alpha]_D^{20}$ -390 (c, 0.2 in $CHCl_3$).

N-*De-Me,* N-*formyl:* ***Nummularine T***
[99694-95-8]
$C_{33}H_{41}N_5O_7$ 619.716
Alkaloid from bark of *Zizyphus nummularia* (Rhamnaceae). Granules (MeOH). Mp 188-190°.

*Dihydro:*Shows antibacterial activity. Needles (CH_2Cl_2/Me_2CO). Mp 281°. $[\alpha]_D^{20}$ -381 (c, 0.15 in MeOH).

Tschesche, R. *et al., Chem. Ber.*, 1974, **107**, 686; 3180 (*isol, uv, ir, pmr, ms, struct*)
Tschesche, R. *et al., Phytochemistry*, 1976, **15**, 541; 1979, **18**, 702 (*isol*)
Pandey, V.B. *et al., Phytochemistry*, 1984, **23**, 2118 (*isol*)
Han, B.H. *et al., Pure Appl. Chem.*, 1989, **61**, 443 (*isol, Nummularine B*)
Pandey, V.B. *et al., Planta Med.*, 1990, **56**, 649 (*activity*)
Singh, B. *et al., Phytochemistry*, 1995, **38**, 271 (*Nummularine T*)

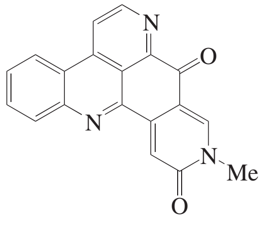
Amphikuemin **A-943**
[105870-54-0]



$C_{16}H_{26}N_3O_3^{\oplus}$ 308.4
Isol. from the sea anenome *Radianthus kuekenthali*. Induces symbiosis between sea anenome and anenome fish.

Murata, M. *et al., Science (Washington, D.C.)*, 1986, **234**, 585-587 (*isol, uv, pmr, struct*)
Konno, K. *et al., Heterocycles*, 1990, **30**, 247-251 (*synth*)

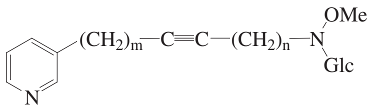
Amphimedine **A-944**
10-Methyl-8H-benzo[b]pyrido[4,3,2-de][1,8]phenanthroline-8,11(10H)-dione, 9CI
[86047-14-5]



$C_{19}H_{11}N_3O_2$ 313.315
Alkaloid from an *Amphimedon* sp. of Pacific sponge and *Xestospongia carbonaria*. Cytotoxic; topoisomerase II inhibitor. Yellow solid. Fairly sol. MeOH; poorly sol. butanol, hexane. Mp 360°. λ_{max} 210 (ϵ 19700); 233 (ϵ 39400); 281 (ϵ 9100); 341 (ϵ 6060) (EtOH) (Derep). λ_{max} 245 (ϵ 38000); 281 (ϵ 10000); 340 (ϵ 7000) (MeOH) (Berdy). λ_{max} 235 (ϵ 38000); 281 (ϵ 10000); 340 (ϵ 7000) (EtOH) (Berdy).

Schmitz, F.J. *et al., J.A.C.S.*, 1983, **105**, 4835 (*isol, uv, ir, pmr, cmr, ms, struct*)
Kubo, A. *et al., Heterocycles*, 1988, **27**, 2095 (*synth, uv, ir, pmr, ms*)
Echavarren, A.M. *et al., J.A.C.S.*, 1988, **110**, 4051 (*synth*)
Prager, R.H. *et al., Aust. J. Chem.*, 1991, **44**, 277 (*synth, uv, ir*)
Guillier, F. *et al., J.O.C.*, 1995, **60**, 292 (*synth*)
Bracher, F. *et al., Annalen*, 1996, 115 (*synth*)
Nakahara, S. *et al., Heterocycles*, 1996, **43**, 2113 (*synth*)

Amphimedoside A **A-945**
[915721-96-9]



m = 4, n = 10

$C_{28}H_{46}N_2O_6$ 506.681
Similar to Hachijodines, H-3. Alkaloid from *Amphimedon* sp. Cytotoxic.

Takekawa, Y. *et al., J. Nat. Prod.*, 2006, **69**, 1503-1505 (*isol, pmr, cmr, ms*)

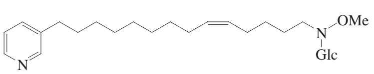
Amphimedoside B **A-946**
[915722-03-1]
As Amphimedoside A, A-945 with
m = 4, n = 8
$C_{26}H_{42}N_2O_6$ 478.628
Alkaloid from *Amphimedon* sp. Cytotoxic.

Takekawa, Y. *et al., J. Nat. Prod.*, 2006, **69**, 1503-1505 (*isol, pmr, cmr, ms*)

Amphimedoside C **A-947**
[915722-04-2]
As Amphimedoside A, A-945 with
m = 2, n = 10
$C_{26}H_{42}N_2O_6$ 478.628
Alkaloid from *Amphimedon* sp. Cytotoxic.

Takekawa, Y. *et al., J. Nat. Prod.*, 2006, **69**, 1503-1505 (*isol, pmr, cmr, ms*)

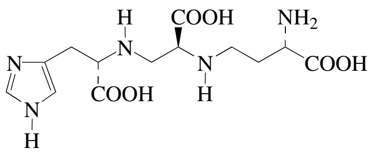
Amphimedoside E **A-948**
[915722-06-4]



$C_{26}H_{44}N_2O_6$ 480.643
Alkaloid from *Amphimedon* sp. Cytotoxic.

Takekawa, Y. *et al., J. Nat. Prod.*, 2006, **69**, 1503-1505 (*isol, pmr, cmr, ms*)

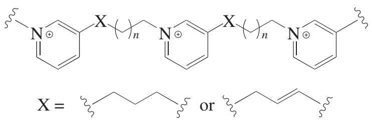
Amphistin **A-949**
[199783-52-3]



$C_{13}H_{21}N_5O_6$ 343.339
Prod. by an actinomycete strain KP-3052. Melanogenesis inhibitor. Powder. Mp 260° (dec.). $[\alpha]_D^{25}$ -9 (c, 0.6 in H_2O). λ_{max} 220 (ϵ 7500) (H_2O).

Arai, N. *et al., J. Antibiot.*, 1997, **50**, 808-814 (*isol, uv, ir, pmr, cmr, N-15 nmr*)

Amphitoxin **A-950**
[165724-12-9]

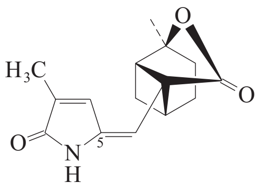


(ratio about 1:1)
n = 5 (mean value)

Polymeric alkaloid from the Caribbean sponge *Amphimedon compressa*. Exhibits antifeedant activity. λ_{max} 266 (H_2O).

Albrizio, S. *et al., J. Nat. Prod.*, 1995, **58**, 647 (*isol, uv, ir, pmr, cmr*)

Ampullicin **A-951**



$C_{15}H_{17}NO_3$ 259.304
Metab. of an *Ampulliferina*-like fungal sp. Needles + ½ H_2O (Me_2CO/C_6H_6/hexane). Mp 197-198°. $[\alpha]_D^{20}$ -32 (c, 0.5 in MeOH). λ_{max} 281 (ϵ 14700) (EtOH) (Derep). λ_{max} 281 (ϵ 14700) (EtOH) (Berdy).

5,6-Dihydro: ***Dihydroampullicin***
[149182-93-4]
$C_{15}H_{19}NO_3$ 261.32
Metab. of an *Ampulliferina*-like fungus. Plant growth regulator. Needles. Sol. MeOH, Me_2CO, EtOAc. Mp 180-181°. $[\alpha]_D^{20}$ +36 (c, 0.25 in MeOH). λ_{max} 244 (ϵ 2490); 248 (ϵ 3000); 254 (ϵ 3350); 260 (ϵ 2400) (EtOH). λ_{max} 244 (ϵ 2940); 248 (ϵ 3000); 254 (ϵ 3350); 260 (ϵ 2400) (EtOH) (Berdy).

5Z-Isomer: ***Isoampullicin***
[127943-13-9]
$C_{15}H_{17}NO_3$ 259.304
From an *Ampulliferina*-like fungal sp. Mp 202-203°. $[\alpha]_D^{20}$ +110 (c, 0.5 in MeOH). λ_{max} 281 (ϵ 14700) (EtOH) (Derep). λ_{max} 284 (ϵ 20500) (EtOH) (Berdy).

Kimura, Y. *et al., Agric. Biol. Chem.*, 1990, **54**, 813 (*isol, pmr, cmr*)
Kimura, Y. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 687-688 (*Dihydroampullicin*)
Rico, R. *et al., Tet. Lett.*, 1995, **36**, 7889-7892; 1996, **37**, 5809-5812 (*synth*)
Marcos, I. *et al., Tet. Lett.*, 2000, **41**, 8451-8455 (*synth, Dihydroampullicin*)
Bermejo, F.A. *et al., J.O.C.*, 2001, **66**, 8287-8292 (*synth, abs config*)

Amsoniaefoline A-952

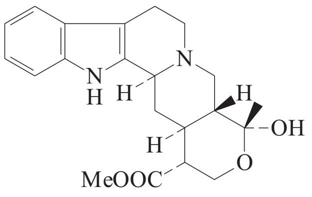
Struct. unknown

$C_{25}H_{32}N_2O_5$ 440.538
Alkaloid from *Rauwolfia amsoniaefolia* (Apocynaceae). Mp 220-223°.

Gomez, R. *et al., J. Philipp. Pharm. Assoc.*, 1957, **44**, 101; 127

Amsosinine A-953

Methyl 19-hydroxy-19-methyloxayohimban-16-carboxylate, 9CI. 19-Hydroxy-16,17-dihydromayumbine
[136092-57-4]



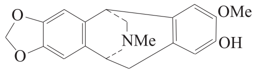
$C_{21}H_{26}N_2O_4$ 370.447
Alkaloid from *Amsonia sinensis* (Apocynaceae). Cryst. Mp 221-222°. $[\alpha]^{14}_{D}$ -51.6 (c, 0.05 in Me_2CO).

16,19-Diepimer: ***Diangoutengjian I***
[344927-27-1]
$C_{21}H_{26}N_2O_4$ 370.447
Alkaloid from *Uncaria yunanensis*. Cryst. (MeOH). Mp 190-191°.

Liu, H.-M. *et al., Planta Med.*, 1991, **57**, 566 (*isol, uv, ir, pmr, cmr, ms, struct*)
Tao, Z.-Y. *et al., Yaoxue Xuebao*, 2001, **36**, 120-122 (*Diangoutengjian I*)

Amurensine† A-954

*10,11-Dihydro-7-methoxy-13-methyl-11,5-(iminomethano)-5*H*-benzo[4,5]cyclohepta[1,2-*f*]-1,3-benzodioxol-8-ol, 9CI. Xanthopetaline*
[10481-92-2]



Absolute configuration

$C_{19}H_{19}NO_4$ 325.363
Alkaloid from *Papaver alpinum, Papaver alpinum* var. *tatricum*, var. *burseri*, var. *kerneri, Papaver pseudocanescens, Papaver nudicaule* var. *amurense*, var. *xanthopetalum*, var. *leiocarpum*, var. *rubroaurantiacum, Papaver pyrenaicum, Papaver tatricum, Papaver suaveolens* and *Papaver anomalum* (Papaveraceae). Cryst. (Me_2CO or MeOH/Et_2O/hexane). Mp 221-223° (206-8°, 213°, 216-217°). $[\alpha]^{22}_{D}$ -178 (c, 0.819 in MeOH). $[\alpha]^{22}_{D}$ -194 (c, 0.25 in $CHCl_3$).

Hydroiodide: Mp 255° dec.

Picrate: Mp 132°.

Me ether: ***Amurensinine***
[10470-47-0]
$C_{20}H_{21}NO_4$ 339.39
Alkaloid from *Papaver tauricola, Papaver anomalum, Papaver pyrenaicum, Papaver pseudocanescens, Papaver alpinum, Papaver alpinum* var. *rhoeaticum*, var. *burseri*, var. *kerneri*, var. *tatricum, Papaver nudicaule* var. *xanthopetalum*, var. *leiocarpum*, var. *rubroaurantiacum, Papaver radicatum* and *Papaver suaveolens* (Papaveraceae). Cryst. (Et_2O or MeOH). Mp 136-138° Mp 144-146° Mp 162-164°. $[\alpha]^{22}_{D}$ -162 (c, 0.80 in $CHCl_3$).

Me ether; hydroiodide:
Cryst. (MeOH/Et_2O). Mp 236-245° dec.

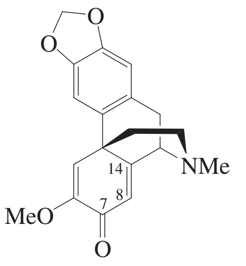
Me ether, N-*oxide(*R-*):* ***Amurensinine N-oxide B***
$C_{20}H_{21}NO_5$ 355.39
Alkaloid from *Meconopsis horridula* var. *racemosa*. $[\alpha]^{27}_{D}$ -89 (c, 0.38 in $CHCl_3$).

Me ether, N-*oxide(*S-*):* ***Amurensinine N-oxide A***
$C_{20}H_{21}NO_5$ 355.39
Alkaloid from *Meconopsis horridula* var. *racemosa*. $[\alpha]^{27}_{D}$ -101 (c, 0.3 in $CHCl_3$).

Boit, H.-G. *et al., Naturwissenschaften*, 1960, **47**, 180 (*isol*)
Maturová, M. *et al., Planta Med.*, 1962, **10**, 345; 1966, **14**, 22 (*isol*)
Šantavý, F. *et al., Chem. Comm.*, 1966, 36; 144
Šantavý, F. *et al., Coll. Czech. Chem. Comm.*, 1966, **31**, 4286 (*uv, ir, pmr, struct*)
Dolejš, L. *et al., Coll. Czech. Chem. Comm.*, 1968, **33**, 600 (*ms*)
Pfeifer, S. *et al., Pharmazie*, 1968, **23**, 585 (*isol, uv*)
Shamma, M. *et al., Tet. Lett.*, 1971, 3425 (*uv, cd*)
Pfeifer, S. *et al., Pharmazie*, 1972, **27**, 48 (*isol, uv, pmr, ms*)
Novák, V. *et al., Coll. Czech. Chem. Comm.*, 1974, **39**, 883 (*isol, uv*)
Böhm, V.H. *et al., Planta Med.*, 1975, **28**, 210 (*isol*)
Dyke, S.F. *et al., Tetrahedron*, 1978, **34**, 241 (*cd*)
Sariyar, G. *et al., Phytochemistry*, 1980, **19**, 2189 (*isol, ms*)
Carrillo, L. *et al., J.O.C.*, 1997, **62**, 6716-6721 (*Amurensinine, synth*)
Xie, H. *et al., Fitoterapia*, 2001, **72**, 120-123 (*Amurensinine N-oxides*)
Tambar, U.K. *et al., J.A.C.S.*, 2006, **128**, 11752-11753 (*Amurensinine, synth*)

Amurine A-955

5,6,8,14-Tetradehydro-6-methoxy-17-methyl-2,3-[methylenebis(oxy)]morphinan-7-one, 9CI



(+)-*form*

$C_{19}H_{19}NO_4$ 325.363

(+)-*form* [4984-99-0]
Alkaloid from *Papaver* spp., esp. *Papaver nudicaule* (Papaveraceae). Cryst. (Me_2CO). Mp 213-215°. $[\alpha]^{26}_{D}$ +10 (c, 1.0 in $CHCl_3$). λ_{max} 238 (log ϵ 3.67); 290 (log ϵ 3.7) (EtOH).

N-*De-Me:* Synthetic. Oil. $[\alpha]^{25}_{D}$ +29.6 (c, 0.3 in $CHCl_3$).

7α-Alcohol: ***Nudaurine***. *Amurinol I*
[4850-04-8]
$C_{19}H_{21}NO_4$ 327.379
Alkaloid from *Papaver nudicaule* var. *aurantiacum* and *Papaver croceum* (Papaveraceae). Cryst. (Me_2CO). Mp 201-202°. $[\alpha]^{22}_{D}$ -52 (c, 1 in $CHCl_3$). Abs. config. revised in 1993. λ_{max} 244 (log ϵ 4); 292 (log ϵ 3.78) (EtOH).

7α-Alcohol, hydroiodide: Mp 198° dec.

7α-Alcohol, picrate: Mp 150° dec.

8,14β-Dihydro, 7α-alcohol: ***Dihydronudaurine***
$C_{19}H_{23}NO_4$ 329.395
Alkaloid from aerial parts of *Papaver pilosum*. Noncryst. $[\alpha]^{20}_{D}$ +100 (c, 0.32 in $CHCl_3$). Incorrectly indexed in CA. λ_{max} 233 (log ϵ 3.97); 292 (log ϵ 3.85) (MeOH).

(-)-*form* [77449-68-4]
Alkaloid from *Roemeria refracta* and *Stephania aculeata*. Amorph. $[\alpha]_{D}$ -14 (c, 0.11 in MeOH). $[\alpha]_{D}$ -10 (c, 0.15 in $CHCl_3$). λ_{max} 242 (log ϵ 4.18); 291 (log ϵ 3.87) (MeOH).

N-*De-Me:* ***Noramurine***
[132209-25-7]
$C_{18}H_{17}NO_4$ 311.337
Alkaloid from *Roemeria refracta* (Papaveraceae). Amorph. $[\alpha]_{D}$ -8 (c, 0.1 in $CHCl_3$). $[\alpha]^{25}_{D}$ -33.3 (c, 0.3 in $CHCl_3$) (synthetic). λ_{max} 240 (log ϵ 4.08); 290 (log ϵ 3.84) (MeOH).

(±)-*form* [21124-18-5]
Yellowish oil.

N-*Me:*
Cryst. (MeOH) (as iodide). Mp 230-233° (222-224°, 202-206° dec.) (iodide).

7α-Alcohol: ***(±)-Nudaurine***. *Alkaloid PN1*
Alkaloid from *Papaver nudicaule* ssp. *xanthopetalum* and *Papaver nudicaule* ssp. *album* (Papaveraceae). Needles (MeOH). Mp 116-117°. Suggested struct. λ_{max} 215 (log ϵ 4.23); 245 (sh) (log ϵ 3.95); 294 (log ϵ 3.91) (MeOH).

8,14ξ-Dihydro: ***8,14-Dihydroamurine***
[1012311-30-6]
$C_{19}H_{21}NO_4$ 327.379
Alkaloid from *Papaver nudicaule*. Amorph. solid. Racemic. λ_{max} 222 (log ϵ 3.79); 254 (log ϵ 3.66); 268 (log ϵ 3.5); 280 (log ϵ 3.49) (MeOH).

Snatzke, G. *et al., J.C.S.(C)*, 1966, 1681-1685 (*cd*)
Döpke, W. *et al., Tetrahedron*, 1968, **24**, 4459-4476 (*struct, pmr*)
Kametani, T. *et al., J.C.S.(C)*, 1969, 801; 1971, 2446-2448; 2712-2714 (*synth*)
Kotani, E. *et al., Tet. Lett.*, 1973, 4759-4762 (*synth*)
Horii, Z. *et al., Chem. Pharm. Bull.*, 1974, **22**, 583-586 (*synth*)
Roblot, F. *et al., Bull. Soc. Chim. Fr.*, 1984, 139-141 (*cmr*)

Vezník, F. *et al., Coll. Czech. Chem. Comm.*, 1985, **50**, 1745-1752; 1987, **52**, 1634-1640 (*Amurine, Alkaloid PN1, isol*)

Gozler, B. *et al., J. Nat. Prod.*, 1990, **53**, 986-988 (*isol, pmr, struct, cd, abs config*)

Gollwitzer, J. *et al., Nat. Prod. Lett.*, 1993, **2**, 197-201 (*Nudaurine, cryst struct, abs config*)

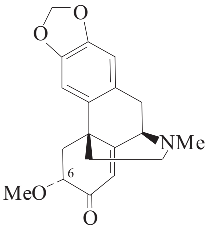
Hara, H. *et al., Tetrahedron: Asymmetry*, 1995, **6**, 1683-1692 (*Amurine, Noramurine, synth*)

Blanchfield, J.T. *et al., Phytochemistry*, 2003, **63**, 711-720 (*(-)-Amurine, isol, pmr, cmr, cryst struct*)

Philipov, S. *et al., Nat. Prod. Res.*, 2007, **21**, 852-856 (*8,14-Dihydroamurine*)

Amurinine A-956

[87245-86-1]



$C_{19}H_{21}NO_4$ 327.379

Alkaloid from the aerial parts of *Papaver pilosum* and *Papaver apokrinomenon* (Papaveraceae). $[\alpha]_D^{20}$ +42 (c, 0.18 in $CHCl_3$). $[\alpha]_D^{20}$ +42 (c, 0.18 in MeOH).

6-Epimer: ***Epiamurinine***

[87220-76-6]

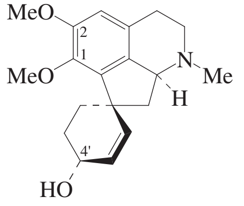
$C_{19}H_{21}NO_4$ 327.379

Alkaloid from the aerial parts of *Papaver pilosum* and *Papaver apokrinomenon* (Papaveraceae). $[\alpha]_D^{20}$ -68 (c, 0.58 in $CHCl_3$).

Hocquemiller, R. *et al., J. Nat. Prod.*, 1984, **47**, 342 (*isol, uv, ir, pmr, ms, struct*)

Oztekin, A. *et al., J. Nat. Prod.*, 1984, **47**, 560 (*isol*)

Amuroline A-957



(+)-*form*

$C_{19}H_{25}NO_3$ 315.411

Diastereomeric with Cryprochine, C-781.

(+)-*form* [10214-57-0]

Alkaloid from *Papaver nudicaule* var. *amurense* (Papaveraceae). Prisms (Me_2CO). Mp 165-166°. $[\alpha]_D^{26}$ +106 (c, 0.3 in $CHCl_3$).

Perchlorate: Mp 151-153°.

Ac: Mp 152-154°. $[\alpha]_D^{24}$ +147 (c, 0.85 in $CHCl_3$).

4-Ketone: ***Amuronine***

[10214-56-9]

$C_{19}H_{23}NO_3$ 313.396

Alkaloid from *Papaver nudicaule* var. *amurense* (Papaveraceae). Mp 119-120° Mp 132-133° (double Mp). $[\alpha]_D^{26}$ +140 (c, 0.3 in $CHCl_3$).

4-Ketone, O^1*-de-Me:* **N-*Methylisocrotsparinine***

$C_{18}H_{21}NO_3$ 299.369

Alkaloid from *Croton sparsiflorus* (Euphorbiaceae). Mp 197-199°. $[\alpha]_D$ +111.5 (c, 0.34 in MeOH).

4-Ketone, O^1*-de-Me,* N*-de-Me:* ***Isocrotsparinine***

[58166-01-1]

$C_{17}H_{19}NO_3$ 285.342

Alkaloid from the aerial parts of *Croton sparsiflorus* (Euphorbiaceae). Cryst. (EtOAc). Mp 198-199°. $[\alpha]_D$ +112.5 (c, 0.23 in $CHCl_3$).

4-Ketone, O^2*-de-Me:* ***Linearisine***

[10214-55-8]

$C_{18}H_{21}NO_3$ 299.369

Alkaloid from *Croton linearis* (Euphorbiaceae). Mp 219-222°. $[\alpha]_D^{28}$ +116 (c, 0.83 in MeOH).

4-Ketone, O^2*-de-Me, hydrochloride:* Mp 300° dec.

10-Epimer, O*-de-Me (?):* ***Discolorine***

$C_{18}H_{23}NO_3$ 301.385

Alkaloid from *Croton discolor* (Euphorbiaceae). Mp 206-208°. $[\alpha]_D$ +99 (c, 0.5 in EtOH). Struct. assigned here on the basis of later work on the stereochem. of these alkaloids. The Me ether was not the same as Amuronine, but MnO_2 oxidn. of the Me ether gave Amuronine (incl. opt. rotn.).

(±)-*form*

Synthetic. Noncryst.

Hydrochloride:

Cryst. ($MeOH/Et_2O$). Mp 235° dec. (preheated to 230°).

Boit, H.-G. *et al., Naturwissenschaften*, 1959, **46**, 514 (*isol*)

Haynes, L.J. *et al., J.C.S.*, 1963, 1784-1788; 1789-1793 (*Linearisine, Amuronine, isol, uv, ir, pmr*)

Haynes, L.J. *et al., J.C.S.(C)*, 1966, 1676-1679 (*Linearisine, Amuronine, struct*)

Snatzke, G. *et al., J.C.S.(C)*, 1966, 1681-1685 (*cd, abs config*)

Baldwin, M. *et al., J.C.S.(C)*, 1967, 154-161 (*ms*)

Bernauer, K. *et al., Helv. Chim. Acta*, 1968, **51**, 1119 (*synth*)

Döpke, W. *et al., Tetrahedron*, 1968, **24**, 2297 (*pmr, cd, struct, stereochem*)

Slavík, J. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 1558 (*ord*)

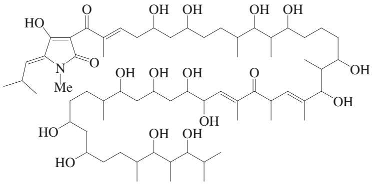
Stuart, K.L. *et al., J.C.S.(C)*, 1970, 1228-1230 (*Discolorine*)

Dolejš, L. *et al., Coll. Czech. Chem. Comm.*, 1974, **39**, 571 (*ms*)

Casagrande, C. *et al., J.C.S. Perkin 1*, 1975, 1659-1663 (*Isocrotsparinine, N-Methylisocrotsparinine*)

Amycomycin A-958

[344362-08-9]



$C_{65}H_{115}NO_{18}$ 1198.619

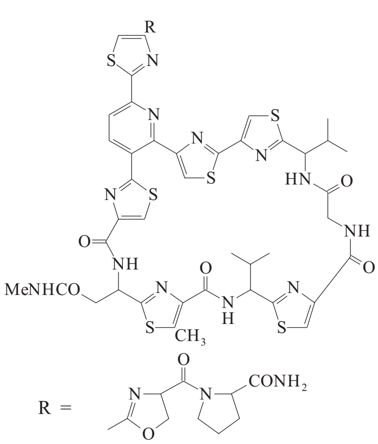
Tetramic acid antibiotic. Prod. by *Amycolatopsis* sp. ST101170. Active against gram-positive bacteria. Amorph. solid. λ_{max} 229 (log ε 3.29); 281 (log ε 3.16) (no solvent reported).

Eur. Pat., 2001, 1 106 604; *CA*, **135**, 32809t (*isol*)

Amythiamicin A A-959

MI 481-42F4A. Antibiotic MI 481-42F4A

[152741-89-4]



$C_{50}H_{51}N_{15}O_8S_6$ 1182.445

CycliC thiazole peptide. Prod. by *Amycolatopsis* sp. MI 481-42F4. Active against gram-positive bacteria. Sol. MeOH, DMSO; poorly sol. H_2O, hexane. $[\alpha]_D^{28}$ +133 (c, 0.7 in DMSO). λ_{max} 203 (ε 83200); 221 (ε 77600); 250 (ε 53700); 310 (ε 35500); 345 (ε 13500) (MeOH) (Derep). λ_{max} 203 (ε 85113); 223 (ε 79432); 303 (ε 33884) (MeOH/HCl). λ_{max} 204 (ε 288400); 309 (ε 33880) (MeOH/NaOH).

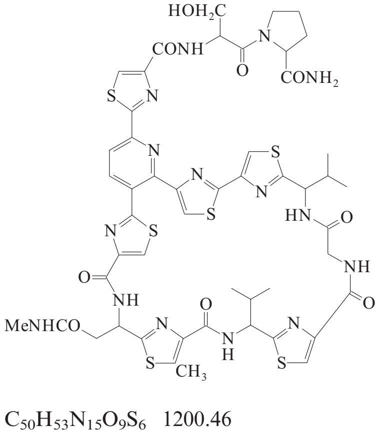
Shimanaka, K. *et al., J. Antibiot.*, 1994, **47**, 668-674; 1145-1152; 1153-1159 (*isol, uv, ir, pmr, cmr, props*)

Nicolaou, K.C. *et al., Chem. Comm.*, 2008, 2632-2634 (*synth*)

Amythiamicin B A-960

MI 481-42F4B. Antibiotic MI 481-42F4B

[156620-48-3]



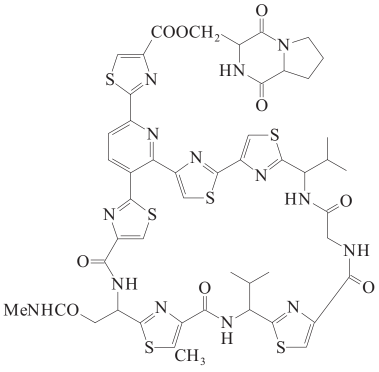
$C_{50}H_{53}N_{15}O_9S_6$ 1200.46

Cyclic polythiazole peptide. Prod. by *Amycolatopsis* sp. MI 481-42F4. Active against gram-positive bacteria. Sol. MeOH, DMSO; poorly sol. H_2O, hexane. $[\alpha]_D^{23}$ +155 (c, 0.25 in MeOH). Nontoxic. λ_{max} 203 (ϵ 83200); 221 (ϵ 77600); 250 (sh) (ϵ 52500); 308 (ϵ 35500); 345 (sh) (ϵ 13500) (MeOH) (Derep). λ_{max} 204 (ϵ 58884); 222 (ϵ 56234); 308 (ϵ 23988) (MeOH/HCl).

Shimanaka, K. *et al., J. Antibiot.*, 1994, **47**, 668-674; 1145-1152; 1153-1159 (*isol, uv, ir, pmr, cmr, props*)
Nicolaou, K.C. *et al., Chem. Comm.*, 2008, 2632-2634 (*synth*)

Amythiamicin C **A-961**

MI 481-42F4C. Antibiotic MI 481-42F4C
[156620-47-2]



$C_{50}H_{50}N_{14}O_9S_6$ 1183.429
Cyclic polythiazole peptide. Prod. by *Amycolatopsis* sp. MI 481-42F4. Active against gram-positive bacteria. Poorly sol. H_2O, hexane. $[\alpha]_D^{24}$ +112 (c, 0.25 in MeOH). λ_{max} 203 (ϵ 83200); 221 (ϵ 77600); 250 (sh) (ϵ 52500); 308 (ϵ 35500); 345 (sh) (ϵ 13500) (MeOH) (Derep). λ_{max} 203 (ϵ 60256); 221 (ϵ 57543); 306 (ϵ 25700) (MeOH/HCl). λ_{max} 203 (ϵ 27542); 306 (ϵ 24547) (MeOH/NaOH).

Shimanaka, K. *et al., J. Antibiot.*, 1994, **47**, 668-674; 1145-1152; 1153-1159 (*isol, uv, ir, pmr, cmr, props*)
Nicolaou, K.C. *et al., Chem. Comm.*, 2008, 2632-2634 (*synth*)

Amythiamicin D **A-962**

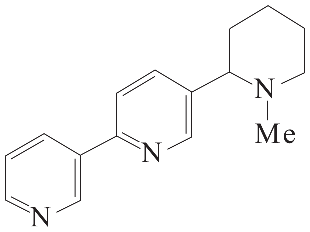
MI 481-42F4D. Antibiotic MI 481-42F4D
[156620-46-1]
As Amythiamicin A, A-959 with
R = –COOMe

$C_{43}H_{42}N_{12}O_7S_6$ 1031.277
Cyclic polythiazole peptide.
Prod. by *Amycolatopsis* sp. MI 481-42F4. Active against gram-positive bacteria. Sol. MeOH, DMSO; poorly sol. H_2O, hexane. $[\alpha]_D^{22}$ +179 (c, 0.5 in MeOH). λ_{max} 204 (ϵ 52500); 224 (ϵ 61700); 250 (sh) (ϵ 36300); 307 (ϵ 30900); 345 (sh) (ϵ 11000) (MeOH) (Derep). λ_{max} 205 (ϵ 52480); 224 (ϵ 63095); 307 (ϵ 31622) (MeOH/HCl). λ_{max} 204 (ϵ 60260); 224 (ϵ 61660); 308 (ϵ 30900) (MeOH/NaOH).

Shimanaka, K. *et al., J. Antibiot.*, 1994, **47**, 668-674; 1145-1152; 1153-1159 (*isol, uv, ir, pmr, cmr, props*)
Hughes, R.A. *et al., J.A.C.S.*, 2005, **127**, 15644-15651 (*synth*)

Anabasamine **A-963**

5-(1-Methyl-2-piperidinyl)-2,3′-bipyridine, 9CI
[20410-87-1]



$C_{16}H_{19}N_3$ 253.346
Alkaloid from the seeds of *Anabasis aphylla* (Chenopodiaceae). Mp 65-66°. $[\alpha]_D$ +107 (c, 3.65 in EtOH).

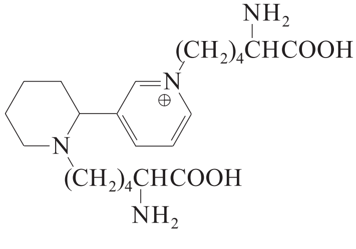
▶ BV4299600

N-*De-Me: 1′′,2′′,3′′,4′′,5′′,6′′-Hexahydro-2,3′:5,2′′-terpyridine. 5-(2-Piperidinyl)-2,3′-bipyridine.* ***Noranabasamine***
[85365-52-2]
$C_{15}H_{17}N_3$ 239.319
Minor alkaloid from skin extracts of the Colombian poison-dart frog *Phyllobates terribilis.* Also identified by gc-ms in skin extracts of *Phyllobates aurotaenia* and *Phyllobates bicolor.* $[\alpha]_D^{25}$ -14.4 (MeOH).

Sadykov, A.S. *et al., Dokl. Akad. Nauk SSSR*, 1967, **24**, 34; *CA*, **68**, 78473e (*isol, uv, ir, pmr, ms, struct*)
Mukhamedzhanov, S.Z. *et al., Khim. Prir. Soedin.*, 1968, **4**, 158; *Chem. Nat. Compd. (Engl. Transl.)*, 1968, **4**, 136 (*uv, ir, pmr, ms, struct*)
Tokuyama, T. *et al., Tetrahedron*, 1983, **39**, 41 (*Noranabasamine*)

Anabilysine **A-964**

1-(1-Amino-1-carboxypentyl)-3-[1-(1-amino-1-carboxypentyl)-2-piperidinyl]-pyridinium(1+)
[66517-63-3]

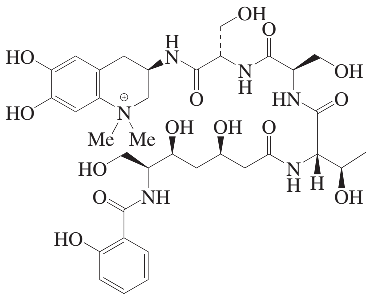


$C_{22}H_{37}N_4O_4^{\oplus}$ 421.559
Isol. from acid hydrolysates of glutaraldehyde-treated ovalbumin. CAS no. refers to chloride. λ_{max} 263 (ϵ 400) (NH_4OH).

Hardy, P.M. *et al., J.C.S. Perkin 1*, 1979, 2282 (*isol, struct, synth, pmr, cmr*)

Anachelin H **A-965**

[326490-92-0]



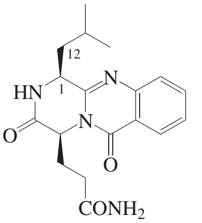
Absolute Configuration

$C_{35}H_{51}N_6O_{14}^{\oplus}$ 779.82
Isol. from *Anabaena cylindrica* CCAP 1403/2A. Siderophore.

Beiderbeck, H. *et al., Z. Naturforsch., C*, 2000, **55**, 681-687 (*isol*)
Gademann, K. *et al., J.O.C.*, 2007, **72**, 8361-8370 (*synth*)

Anacine **A-966**

[154613-22-6]



Absolute Configuration

$C_{18}H_{22}N_4O_3$ 342.397
Struct. revised in 1999. Related to Fumiquinazoline A, F-185. Metab. of marine-derived and terrestrial *Penicillium aurantiogriseum*. Also from *Penicillium polonicum*. Mycotoxin. Amorph. solid. Sol. H_2O; poorly sol. Me_2CO, hexane. $[\alpha]_D^{24}$ +233.3 (c, 0.21 in MeOH). λ_{max} 226 (log ϵ 4.23); 270 (log ϵ 3.6) (MeOH).

*1,12-Didehydro(*Z-*):* ***Aurantiomide C***
[915190-86-2]
$C_{18}H_{20}N_4O_3$ 340.381
Prod. by the marine-derived *Penicillium aurantiogriseum* SP0-16. Amorph. powder. $[\alpha]_D^{24}$ +25.8 (c, 0.1 in $CHCl_3$). λ_{max} 314 (log ϵ 4.48) (MeOH).

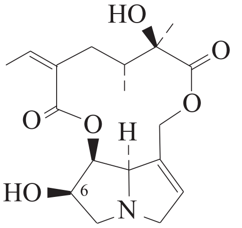
1-Hydroxy: ***Aurantiomide B***
[915190-84-0]
$C_{18}H_{22}N_4O_4$ 358.396
Prod. by the marine-derived *Penicillium aurantiogriseum* SP0-19. Amorph. powder. $[\alpha]_D^{24}$ +96.5 (c, 0.09 in $CHCl_3$). $[\alpha]_D$ +172 (c, 1.8 in MeOH). λ_{max} 280 (log ϵ 4.6); 311 (log ϵ 4.28) (MeOH).

1-Methoxy: ***Aurantiomide A***
[915190-85-1]
$C_{19}H_{24}N_4O_4$ 372.423
Prod. by the marine-derived *Penicillium aurantiogriseum* SP0-19. Oil. $[\alpha]_D^{24}$ +16 (c, 0.05 in $CHCl_3$). λ_{max} 282 (log ϵ 3.9); 311 (log ϵ 3.71) (MeOH).

Boyes-Korkis, J.M. *et al., J. Nat. Prod.*, 1993, **56**, 1707-1717 (*isol, uv, ir, pmr, cmr, ms*)
Larsen, T.O. *et al., J. Nat. Prod.*, 1999, **62**, 1578-1580 (*struct*)
Wang, H. *et al., J. Nat. Prod.*, 2001, **64**, 1497-1501 (*synth, pmr, cmr*)
Xin, Z.H. *et al., J. Nat. Prod.*, 2007, **70**, 853-855 (*Aurantiomides A-C*)

Anacrotine A-967

6,12-Dihydroxysenecionan-11,16-dione, 9CI. Crotalaburnine
[5096-49-1]



Absolute configuration

$C_{18}H_{25}NO_6$ 351.399

Cyclic diester of Crotanecine, C-775 with senecic acid. Alkaloid from *Crotalaria laburnifolia* (Fabaceae). Mp 191-192°. $[\alpha]_D$ +30 (EtOH).

▶ Hepato- and pneumotoxin. VT5707000

O^6-*Ac:* ***Acetylanacrotine***
$C_{20}H_{27}NO_7$ 393.436
Alkaloid from *Crotalaria agatiflora* (Fabaceae). Mp 106-107°. $[\alpha]_D$ +74 (c, 0.4 in EtOH).

6-Epimer: ***Uspallatine***
[98264-41-6]
Alkaloid from the roots of *Senecio uspallatensis* (Asteraceae). Cryst. (MeOH/CHCl$_3$). Mp 205-207°. $[\alpha]_D^{20}$ +4.11 (c, 0.0764 in MeOH).

*(*E*)-Isomer:* **trans-*Anacrotine***
$C_{18}H_{25}NO_6$ 351.399
Minor alkaloid from seeds of *Crotalaria capensis* (Fabaceae). $[\alpha]_D^{22}$ +11 (c, 1.7 in CHCl$_3$).

*(*E*)-Isomer,* O^6-*Ac:* ***Acetyl*-trans-*anacrotine***
$C_{20}H_{27}NO_7$ 393.436
Alkaloid from *Crotalaria agatiflora* (Fabaceae). Prisms (EtOH). Mp 96-97°. $[\alpha]_D$ +65 (c, 1.37 in EtOH).

*(*E*)-Isomer,* O^6*-angeloyl,* N*-oxide:* ***Angeloyl*-trans-*anacrotine* N*-oxide***
$C_{23}H_{31}NO_8$ 449.5
Alkaloid from *Crotalaria agatiflora* (Fabaceae). Mp 175-176°.

Atal, C.K. *et al., Tet. Lett.*, 1966, 537 (*isol, struct, pmr*)
Culvenor, C.C.J. *et al., An. Quim.*, 1972, **68**, 883 (*derivs*)
Crout, D.H.G. *et al., J.C.S. Perkin 1*, 1972, 1602 (*isol*)
Culvenor, C.C.J. *et al., Chem. Biol. Interact.*, 1976, **12**, 299 (*tox*)
Jones, A.J. *et al., Aust. J. Chem.*, 1982, **35**, 1173 (*cmr*)
Mackay, M.F. *et al., Acta Cryst. C*, 1984, **40**, 1073 (*cryst struct*)
Pestchanker, M.J. *et al., Phytochemistry*, 1985, **24**, 1622 (*Uspallatine*)
Verdoorn, G.H. *et al., Phytochemistry*, 1992, **31**, 369 (*trans-Anacrotine*)

Anacycline A-968

N*-(2-Methylpropyl)-2,4-tetradecadiene-8,10-diynamide, 9CI. 2,4-Tetradecadiene-8,10-diynoic acid isobutylamide*
[502-57-8]
$H_3CCH_2CH_2C{\equiv}CC{\equiv}CCH_2CH_2CH{=}CHCH{=}CHCONHCH_2CH(CH_3)_2$

$C_{18}H_{25}NO$ 271.402
λ_{max} 230 (ϵ 10000); 259 (ϵ 33500); 265 (sh) (ϵ 29800) (EtOH) (Derep).

(E,E)-form [94413-18-0]
Alkaloid from the roots of *Anacyclus pyrethrum* (Asteraceae) and *Achillea* spp. Cryst. (Et$_2$O/petrol). Mp 122°.

Maleic anhydride adduct:
Cryst. (Et$_2$O/petrol). Mp 196°.

N*-Me:* N*-Methyl-*N*-(2-methylpropyl)-2,4-tetradecadiene-8,10-diynamide.* **N*-Methylanacycline***
[38340-83-9]
$C_{19}H_{27}NO$ 285.428
Constit. of the roots of *Anacyclus pyrethrum* (Asteraceae). Oil. λ_{max} 251 nm.

Tetrahydro:
Waxy needles. Mp 40°.

12,13-Didehydro: N*-Isobutyl-2,4,12-tetradecatriene-8,10-diynamide. Dehydroanacycline. 12,13-Didehydroanacycline*
[29428-83-9]
$C_{18}H_{23}NO$ 269.386
Alkaloid from *Anacyclus fuscata* and *Achillea* spp. (Asteraceae). Cryst. (petrol). Mp 150.5°. Becomes rose-pink on prolonged exposure to sunlight.

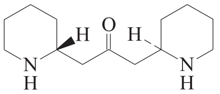
(E,Z)-form [37064-16-7]
Synthetic. Cryst. (Et$_2$O/petrol). Mp 85.5°.

[112711-13-4 , 94481-83-1]

Crombie, L. *et al., J.C.S.*, 1955, 999 (*isol, uv, ir, struct*)
Bohlmann, F. *et al., Chem. Ber.*, 1956, **89**, 1276; 1970, **103**, 2856; 1974, **107**, 2120 (*synth, biosynth, uv, ir, Didehydroanacycline*)
Crombie, L. *et al., Chem. Ind. (London)*, 1956, 409 (*synth, uv*)
Crombie, L. *et al., J.C.S.*, 1957, 2767 (*synth*)
Jente, R. *et al., Chem. Ber.*, 1972, **105**, 1694 (*isol, synth, ir, pmr, uv*)
Kuropka, G. *et al., Planta Med.*, 1987, **53**, 440 (*isol*)
Crombie, L. *et al., Tet. Lett.*, 1987, **28**, 4875 (*synth*)
Greger, H. *et al., Phytochemistry*, 1989, **28**, 2363 (*isol*)

Anaferine A-969

1,3-Di-2-piperidinyl-2-propanone, 9CI



(R,R)−form

$C_{13}H_{24}N_2O$ 224.345

The isolated alkaloid is the *meso*-form, but Anaferine readily racemises and the (±)-form epimerises to the *meso*-form in aq. soln., so it is probable that the nat. alkaloid is opt. active.

(R,R)-form [19519-55-2]
[19519-54-1 dihydrobromide]
Mp 242.5-243.5° (as dihydrochloride). $[\alpha]_D^{22}$ -49.8 (c, 0.529 in MeOH) (dihydrochloride).

(S,S)-form [19519-53-0]
[19519-52-9 dihydrochloride]
Mp 242.5-244° (as dihydrochloride). $[\alpha]_D^{22}$ +50.7 (c, 0.736 in MeOH) (dihydrochloride).

(RS,RS)-form
(±)-form
[28666-51-5]

Dihydrobromide: Mp 247-249°.

Dipicrate: Mp 177-179°.

(RS,SR)-form
meso*-form*
[28699-15-2]
Constit. of root of *Withania somnifera* (Solanaceae). Mp 16-17°. Bp$_{0.01}$ 55°.

Dihydrochloride: Mp 226-228°.

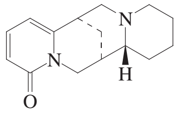
Dihydrobromide: Mp 227-229°.

Dipicrate: Mp 180-182° Mp 193-195° (dimorph.).

Rother, A. *et al., Chem. Ind. (London)*, 1962, 654 (*isol, ir, ms, pmr, struct*)
Schöpf, C. *et al., Annalen*, 1970, **737**, 1 (*synth, ir, abs config*)
Beyerman, H.C. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1971, **90**, 1326 (*abs config*)
Cymerman Craig, J. *et al., J.O.C.*, 1978, **48**, 347 (*ord, cd*)
Blechert, S. *et al., Eur. J. Org. Chem.*, 2002, 2855-2858 (*synth, abs config*)

Anagyrine A-970

*7,7*a*,8,9,10,11,13,14-Octahydro-7,14-methano-4*H*,6*H*-dipyrido[1,2-*a*;1′,2′-*e*][1,5]diazocin-4-one, 9CI. Rhombinine. Monolupine. Alkaloid III*
[486-89-5]
[34389-11-2 ((±)-form)]



Absolute Configuration

$C_{15}H_{20}N_2O$ 244.336

Alkaloid from *Anagyris foetida*, several *Cytisus*, *Genista*, *Lupinus*, *Sophora* and *Ammodendron* spp, *Ulex europaeus*, *Ulex nanus*, *Templetonia retusa* and *Thermopsis chinensis.* Antiarrhythmic, diuretic, purgative agent. Cardiotonic agent inducing tachycardia. Major toxic alkaloid responsible for "crooked calf disease" caused by leguminous plants. Noncryst. $[\alpha]_D$ -165 (EtOH). Log P 0.82 (calc). A reported crystal structure determination (1991) of Anagyrine was erroneous; it was Thermopsine, T-363.

▶ Exp. teratogen. BV5620000

Hydrochloride: Mp 295-297°.

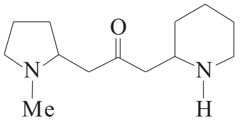
Methiodide: Mp 264° dec.

Hydroxy: ***Hydroxyanagyrine***
[67984-05-8]
$C_{15}H_{20}N_2O_2$ 260.335
Alkaloid from *Anagyris foetida* (Fabaceae). No phys. props. reported. Substd. in the D-ring (ring remote from the carbonyl function); posn. of subn. unknown.

11-Epimer: see Thermopsine, T-363

Couch, J.F. *et al., J.A.C.S.*, 1939, **61**, 3327 (*isol*)
Ribas, I. *et al., An. R. Soc. Esp. Fis. Quim., Ser. B*, 1952, **48**, 161; 167 (*isol*)
van Tamelen, E.E. *et al., J.A.C.S.*, 1958, **80**, 4659 (*synth*)
Fales, H.M. *et al., J.A.C.S.*, 1970, **92**, 1590 (*ms*)
Goldberg, S.I. *et al., J.O.C.*, 1972, **37**, 1823 (*synth*)
Bohlmann, F. *et al., Chem. Ber.*, 1975, **108**, 1043 (*cmr*)
Keeler, R.F. *et al., CA*, 1976, **85**, 138290f (*tox*)
Lobo, J.M. *et al., An. Quim.*, 1977, **73**, 1366 (*Hydroxyanagyrine*)
Rycroft, D.S. *et al., Magn. Reson. Chem.*, 1991, **29**, 936 (*pmr, cmr, conformn*)
Robins, D.J. *et al., Magn. Reson. Chem.*, 1992, **30**, 1125 (*config*)
Rode, J.E. *et al., J. Mol. Struct.*, 2005, **749**, 1 (*cryst struct*)
Gray, D. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 2419-2423 (*synth*)

Anahygrine A-971



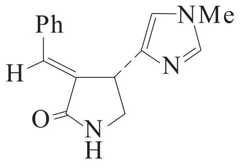
$C_{13}H_{24}N_2O$ 224.345
Alkaloid from roots of *Withania somnifera* (Solanaceae). Pale yellow oil. $Bp_{0.2}$ 106°.

Dihydrochloride: Mp 216.5-217.5°.

Dipicrate: Mp 173-174.5°.

Schwarting, A.E. *et al., J. Nat. Prod.*, 1963, **26**, 258 (*isol*)
Leary, J.D. *et al., Chem. Ind. (London)*, 1964, 283 (*isol*)
El-Olemy, M.M. *et al., Experientia*, 1965, **21**, 249 (*synth*)

Anantine† A-972



$C_{15}H_{15}N_3O$ 253.303
λ_{max} 218 (ϵ 15800); 277 (ϵ 25000) (prob. MeOH) (Derep).

(*R*)-*form* [50656-82-1]
Alkaloid from the leaves of *Cynometra ananta* and from the root bark, trunk bark and leaves of *Cynometra lujae* (Fabaceae). Mp 204°. $[\alpha]_D$ -549.

N-*Ac:* Mp 99°. $[\alpha]_D$ -365.

N-*De-Me:* ***Noranantine***
[85651-90-7]
$C_{14}H_{13}N_3O$ 239.276
Alkaloid from the root bark and trunk bark of *Cynometra lujae* (Fabaceae). Cryst. (Me_2CO/MeOH). Mp 205°. $[\alpha]_D^{20}$ -431 (c, 1 in $CHCl_3$).

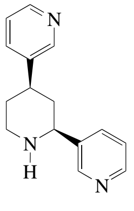
3′-Hydroxy: ***Hydroxyanantine***
[85644-21-9]
$C_{15}H_{15}N_3O_2$ 269.302
Alkaloid from the root bark and trunk bark of *Cynometra lujae* (Fabaceae). Cryst. (Me_2CO/MeOH). Mp 170°. $[\alpha]_D^{20}$ -433 (c, 1 in $CHCl_3$). Hydroxylated in the phenyl ring.

(±)-*form* [68069-26-1]
Synthetic. Mp 179°.

Khuong-Huu, F. *et al., Tet. Lett.*, 1973, 1757 (*ir, uv, pmr, cmr, struct*)
Tchissambou, L. *et al., Tet. Lett.*, 1978, 1801 (*synth*)
Tchissambou, L. *et al., Tetrahedron*, 1982, **38**, 2687 (*isol, cmr, struct, derivs*)
Naito, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1932-1939 (*synth*)

Anatalline A-973

3,3′-(2,4-Dipiperidinediyl)bispyridine, 9CI. 2,4-Di-3-pyridylpiperidine
[18793-19-6]



Relative configuration

$C_{15}H_{17}N_3$ 239.319
Alkaloid from the leaves and roots of *Nicotiana tabacum*. Also found in *Duboisia hopwoodii*. Amorph. solid. Bp_3 225°. $[\alpha]_D$ 0. Isol. as a mixt. with its *trans*-isomer. Dehydrogenation gives 3,2′:4′,3′′-Terpyridine, T-98.

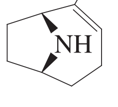
Perchlorate (1:3): [18793-18-5]
Cryst. (MeOH/Et_2O). Mp 244-252°.

Picrate: [18793-20-9]
Mp 258.5°.

Kisaki, T. *et al., Phytochemistry*, 1968, **7**, 323-327 (*isol, ir, pmr, ms*)
Rao, H.S.P. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 557-561 (*synth, pmr, cmr, config*)
Häkkinen, S.T. *et al., Planta Med.*, 2004, **70**, 936-941 (*isol, pmr, cmr, ms*)

Anatoxin a A-974

1-(9-Azabicyclo[4.2.1]non-2-en-2-yl)ethanone, 9CI. 2-Acetyl-9-azabicyclo[4.2.1]non-2-ene. Very fast death factor. VFDF. AnTx



(+)-*form*

$C_{10}H_{15}NO$ 165.235

(+)(HCl)-*form* [64285-06-9]
[64314-16-5 (hydrochloride)]
Alkaloid from *Anabaena flos-aquae* NRC-44h (Euphorbiaceae). Also isol. from *Oscillatoria* spp., *Aphanizomenon flos-aquae* and *Cylindrospermum* sp. Depolarising agent. Potent agonist for the nicotinic acetylcholine receptor. Oil. Sol. H_2O, MeOH. $[\alpha]_D^{24}$ +43.2 (c, 0.676 in EtOH). λ_{max} 226 (ϵ 8300) (MeOH) (Berdy). λ_{max} 227 (ϵ 10000) (EtOH) (Berdy).
▶ Exp. reprod. effects. Very toxic by intraperitoneal route; LD_{50} (mus, ipr) 0.3 mg/kg, LD_{50} (mus, ipr) 0.2 mg/kg. KM5527000

N-*Ac:* Mp 117-118°. $[\alpha]_D$ -127 (c, 4.8 in EtOH).

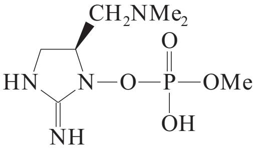
(-)(HCl)-*form* [92142-32-0]
Synthetic. $[\alpha]_D^{23}$ -45 (c, 0.3 in EtOH) (hydrochloride).

Devlin, J.P. *et al., Can. J. Chem.*, 1977, **55**, 1367-1371 (*isol, pmr, cmr, ms*)
Campbell, H.F. *et al., Can. J. Chem.*, 1977, **55**, 1372 (*synth*)
Bates, H.A. *et al., J.A.C.S.*, 1979, **101**, 1259-1265 (*synth*)
Spivak, C.E. *et al., Mol. Pharmacol.*, 1980, **18**, 384-394; 1983, **23**, 337-343; 1986, **29**, 250-257 (*pharmacol*)
Petersen, J.S. *et al., J.A.C.S.*, 1984, **106**, 4539-4547 (*synth*)
Koskinen, A.M.P. *et al., J. Med. Chem.*, 1985, **28**, 1301-1309 (*synth, cryst struct*)
Danheiser, R.L. *et al., J.A.C.S.*, 1985, **107**, 8066 (*synth*)
Tufariello, J.J. *et al., Tetrahedron*, 1985, **41**, 3447 (*synth*)
Wiseman, J.R. *et al., J.O.C.*, 1986, **51**, 2485 (*synth, bibl*)
Vernon, P. *et al., Chem. Comm.*, 1987, 245 (*synth, bibl*)
Stjernloef, P. *et al., Acta Chem. Scand.*, 1989, **43**, 917 (*synth*)
Matsunaga, S. *et al., J.A.C.S.*, 1989, **111**, 8021 (*isol*)
Sardina, F.J. *et al., J.O.C.*, 1989, **54**, 4654; 1990, **55**, 5025 (*synth, bibl*)
Gallon, J.R. *et al., Phytochemistry*, 1990, **29**, 1107; 1994, **35**, 1195 (*biosynth*)
Somfai, P. *et al., Tet. Lett.*, 1992, **33**, 3791 (*synth*)
Skrinjar, M. *et al., Tetrahedron: Asymmetry*, 1992, **3**, 1263 (*synth*)
Harada, K. *et al., Tetrahedron*, 1993, **49**, 9251 (*isol*)
Newcombe, N.J. *et al., Chem. Comm.*, 1995, 831 (*synth*)
Hemscheidt, T. *et al., Chem. Comm.*, 1995, 1361-1362 (*biosynth*)
Molloy, L. *et al., Eur. J. Pharmacol.*, 1995, **289**, 447-453 (*pharmacol*)
Mansell, H.L. *et al., Tetrahedron*, 1996, **52**, 6025 (*rev, synth*)
Parsons, P.J. *et al., Tetrahedron*, 1996, **52**, 11637 (*synth*)
Oh, C.-Y. *et al., Tet. Lett.*, 1998, **39**, 2133-2136 (*synth*)
Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)
Parsons, P.J. *et al., Tetrahedron*, 2000, **56**, 309-315 (*synth*)
Mori, M. *et al., Tet. Lett.*, 2004, **45**, 4397-4399 (*synth*)
Brenneman, J.B. *et al., Tetrahedron*, 2004, **60**, 7301-7314 (*synth*)
Ho, T.-L. *et al., Helv. Chim. Acta*, 2006, **89**, 134-137 (*synth*)

Wonnacott, S. *et al., Mar. Drugs*, 2006, **4**, 228-254 (*rev, activity*)
Tomita, T. *et al., Tetrahedron*, 2006, **62**, 10518-10527 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, AOO120

Anatoxin a(s) A-975

*2-Amino-4,5-dihydro-1-[(hydroxymethoxyphosphinyl)oxy]-*N,N*-dimethyl-1*H*-imidazole-5-methanamine, 9CI*
[103170-78-1]

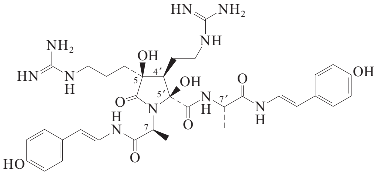


$C_7H_{17}N_4O_4P$ 252.209
Isol. from the blue-green alga, *Anabaena flos-aquae* NRC525.17. Potent neurotoxin with anticholinesterase activity. Dec. slowly at -20°. λ_{max} 200 (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 0.05 mg/kg. BV6593100

Matsunaga, S. *et al., J.A.C.S.*, 1989, **111**, 8021-8023 (*isol, pmr, cmr*)

Anchinopeptolide A A-976

[152369-61-4]



$C_{34}H_{46}N_{10}O_8$ 722.8
Stereochem. at C-5, C-4′ and C-5′ is relative. Isol. from the marine sponge *Anchinoe tenacior*. $[\alpha]_D$ -103.6 (c, 4 in MeOH). λ_{max} 217 (ϵ 13600); 285 (ϵ 20000) (MeOH) (Derep).

7-Demethyl: ***Anchinopeptolide C***
[160041-36-1]
$C_{33}H_{44}N_{10}O_8$ 708.773
From *Anchinoe tenacior*. $[\alpha]_D$ -6.3 (c, 1 in MeOH). λ_{max} 284 (ϵ 14490); 320 (MeOH) (Berdy).

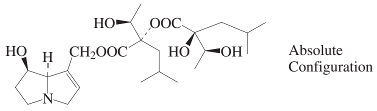
7′-Demethyl: ***Anchinopeptolide B***
[160072-37-7]
$C_{33}H_{44}N_{10}O_8$ 708.773
From *Anchinoe tenacior*. $[\alpha]_D$ -12.4 (c, 0.7 in MeOH). λ_{max} 284 (ϵ 12070); 318 (MeOH) (Berdy).

7,7′-Bis(demethyl): ***Anchinopeptolide D***
[160072-38-8]
$C_{32}H_{42}N_{10}O_8$ 694.746
From *Anchinoe tenacior*. $[\alpha]_D$ +11.4 (c, 1 in MeOH). λ_{max} 284 (ϵ 16940); 318 (MeOH) (Berdy).

Casapullo, A. *et al., Tet. Lett.*, 1993, **34**, 6297 (*isol, uv, ir, pmr, cmr, struct*)
Casapullo, A. *et al., J. Nat. Prod.*, 1994, **57**, 1227 (*Anchinopeptolides B-D*)
Snider, B.B. *et al., J.O.C.*, 2000, **65**, 793-800 (*Anchinopeptolide D, synth*)

Anchustrigosine A-977

[701974-94-9]

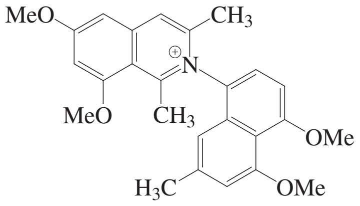


$C_{24}H_{41}NO_8$ 471.59
Alkaloid from the roots of *Anchusa strigosa*. Red oil. $[\alpha]_D^{25}$ -4 (c, 0.1 in MeOH). λ_{max} 239 (sh) ; 286 (MeOH).

Braca, A. *et al., Planta Med.*, 2003, **69**, 835-841 (*isol, pmr, cmr*)

Ancisheynine A-978

[603933-04-6]

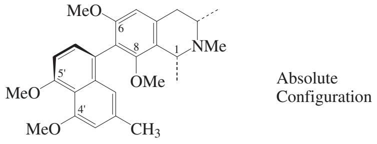


$C_{26}H_{28}NO_4^{\oplus}$ 418.512
Quaternary alkaloid from the aerial parts of *Ancistrocladus heyneanus*. Yellow solid. Counterion not specified. Racemate. λ_{max} 233 (log ϵ 4.47); 264 (log ϵ 4.29); 307 (log ϵ 3.89); 358 (log ϵ 3.71) (MeOH).

Yang, L.-K. *et al., Tet. Lett.*, 2003, **44**, 5827-5829
Bringman, G. *et al., Org. Lett.*, 2006, **8**, 1037-1040 (*synth*)

Ancistrobrevine A A-979

[169276-08-8]



$C_{27}H_{33}NO_4$ 435.562
Alkaloid from *Ancistrocladus abbreviatus* (Ancistrocladaceae).

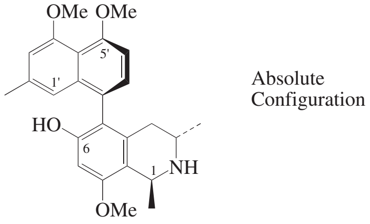
*1-Epimer, 5′,8-di-*O*-de-Me,* N*-de-Me:* ***Ancistrogriffine C***
[478796-16-6]
$C_{24}H_{27}NO_4$ 393.482
Alkaloid from *Ancistrocladus griffithii*. Light yellow powder (MeOH). Mp 165°. $[\alpha]_D^{25}$ +13.8 (c, 0.25 in MeOH).

*Atropisomer, 1-epimer, 4′,6-di-*O*-de-Me:* ***Ancistrogriffine A***
[478796-14-4]
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from *Ancistrocladus griffithii*. Cryst. (MeOH). Mp 148°. $[\alpha]_D^{25}$ +26 (c, 0.4 in MeOH).

Bringmann, G. *et al., Magn. Reson. Chem.*, 1997, **35**, 297-301 (*pmr, config*)
Bringmann, G. *et al., Phytochemistry*, 2002, **61**, 195-204 (*Ancistrogriffines*)

Ancistrobrevine B A-980

[146471-74-1]



$C_{25}H_{29}NO_4$ 407.508
Alkaloid from *Ancistrocladus abbreviatus* and *Ophiopogon japonicus*. Amorph. powder (MeOH/Me_2CO). Mp 122-124°. $[\alpha]_D$ -68 (c, 0.81 in $CHCl_3$).

6-Me ether: ***Ancistrotectoriline A***
[302543-63-1]
$C_{26}H_{31}NO_4$ 421.535
Alkaloid from *Ancistrocladus tectorius*. Amorph. solid. Mp 103-105°. $[\alpha]_D^{25}$ +1.3 (c, 0.75 in $CHCl_3$).

6-Me ether, N*-Me:* ***5-Epi-6-*O*-methylancistrobertsonine A***. N*-Methylancistrotectoriline A*
$C_{27}H_{33}NO_4$ 435.562
Alkaloid from a Congolese *Ancistrocladus* sp. Amorph. solid. $[\alpha]_D^{25}$ +1.2 (c, 0.09 in MeOH). λ_{max} 237 (log ϵ 1.29); 307 (log ϵ 0.4); 321 (log ϵ 0.33); 337 (log ϵ 0.26) (CH_2Cl_2).

*4′,8-Di-*O*-de-Me, 6-Me ether,* N*-Me:*
[222409-76-9]
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from *Ancistrocladus likoko*.

1,2-Didehydro, 6-Me ether: ***Ancistrotanzanine B***
[604767-80-8]
$C_{26}H_{29}NO_4$ 419.519
Alkaloid from *Ancistrocladus likoko* and *Ancistrocladus tanzaniensis*. Yellow oil. $[\alpha]_D^{25}$ +44 (c, 0.01 in MeOH). λ_{max} 230 (log ϵ 1.89); 305 (log ϵ 1.42) (MeOH).

*1-Epimer, 4′-*O*-de-Me, 6-Me ether,* N*-Me:* ***5-Epi-4′-*O*-demethylancistrobertsonine C***
$C_{26}H_{31}NO_4$ 421.535
Alkaloid from a Congolese *Ancistrocladus* sp. Cryst. (MeOH). Mp 92° (synthetic). $[\alpha]_D^{25}$ +15.7 (c, 0.12 in MeOH) (natural). $[\alpha]_D^{20}$ +51.8 (c, 1 in MeOH) (synthetic). λ_{max} 230 (log ϵ 1.05); 307 (log ϵ 0.42) (CH_2Cl_2).

Epimer, 6-Me ether, N*-Me:* [222409-80-5]
$C_{27}H_{33}NO_4$ 435.562
Alkaloid from *Ancistrocladus likoko*. Possesses *cis*-config.

Atropisomer, N*-Me:* ***Ancistrobertsonine A***
$C_{26}H_{31}NO_4$ 421.535
Alkaloid from *Ancistrocladus robertsoniorum* (Ancistrocladaceae). Cryst. (MeOH aq.). Mp 220-222°. $[\alpha]_D^{25}$ +29 (c, 0.5 in $CHCl_3$).

*Atropisomer, 5′-*O*-de-Me:* ***Ancistroguineine A***
[202343-74-6]
$C_{24}H_{27}NO_4$ 393.482
Alkaloid from *Ancistrocladus guineen-*

sis. Needles ($CHCl_3$). Mp 202-204°. $[\alpha]_D^{25}$ +191.4 (c, 0.5 in $CHCl_3$).

*Atropisomer, 5′-*O*-de-Me, 6-Me ether:* ***Ancistroealaine B***
[303752-19-4]
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from *Ancistrocladus ealaensis.* Yellow powder (MeOH). Mp 248°. $[\alpha]_D^{20}$ -16.7 (c, 0.71 in EtOH).

Atropisomer, 1,2-didehydro: ***6-O-Demethylancistroealaine A***
$C_{25}H_{27}NO_4$ 405.493
Alkaloid from a Congolese *Ancistrocladus* sp. Yellow cryst. Mp 155-160°. $[\alpha]_D^{25}$ -63.2 (c, 0.1 in MeOH). λ_{max} 232 (log ε 1.06); 310 (log ε 0.34); 316 (log ε 0.34); 321 (log ε 0.35); 334 (log ε 0.33) (CH_2Cl_2).

Atropisomer, 1,2-didehydro, 6-Me ether: ***Ancistroealaine A***
[303752-18-3]
$C_{26}H_{29}NO_4$ 419.519
Alkaloid from *Ancistrocladus ealaensis.* Light yellow powder (MeOH). Mp 94-96°. $[\alpha]_D^{25}$ -34.3 (c, 0.55 in EtOH).

*Atropisomer, 1,2-didehydro, 4′-*O*-de-Me:* ***Ancistrolikokine D***
$C_{24}H_{25}NO_4$ 391.466
Alkaloid from *Ancistrocladus likoko*. Amorph. solid. Mp 122-124°. $[\alpha]_D^{25}$ +191.6 (c, 0.15 in $CHCl_3$).

*Atropisomer, 1,2-didehydro, 5′-*O*-de-Me:* ***5′,6-Di-O-demethylancistroealaine A***
$C_{24}H_{25}NO_4$ 391.466
Alkaloid from a Congolese *Ancistrocladus* sp. Amorph. yellow solid. $[\alpha]_D^{25}$ -68.6 (c, 0.1 in MeOH). λ_{max} 235 (log ε 1.15); 313 (log ε 0.47); 316 (log ε 0.47); 321 (log ε 0.48); 325 (log ε 0.47); 335 (log ε 0.45) (CH_2Cl_2).

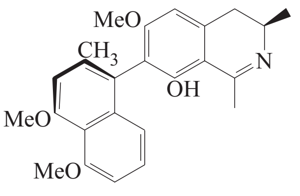
Atropisomer, 1-epimer, 6-Me ether, N*-Me:* ***Ancistrobertsonine C***
[250130-68-8]
$C_{27}H_{33}NO_4$ 435.562
Alkaloid from *Ancistrocladus robertsoniorum*. Mp 148-149°. $[\alpha]_D^{25}$ -3 (c, 0.09 in $CHCl_3$).

*Atropisomer, 3-epimer, 5′-*O*-de-Me:* ***Ancistroguineine B***
[202420-24-4]
$C_{24}H_{27}NO_4$ 393.482
Alkaloid from *Ancistrocladus guineensis.* Amorph. solid. $[\alpha]_D^{25}$ -141.2 (c, 0.04 in $CHCl_3$).

Bringmann, G. *et al., Phytochemistry*, 1992, **31**, 4011; 1998, **47**, 31-35; 37-43; 1999, **52**, 321-332 (*isol, ir, cd, pmr, ms, struct, derivs*)
Bringmann, G. *et al., Phytochemistry*, 1998, **49**, 1667 (*Ancistrorobertsonine A*)
Hoye, T.R. *et al., J.O.C.*, 1999, **64**, 7184-7201 (*synth*)
Bringmann, G. *et al., Magn. Reson. Chem.*, 1999, **37**, 98-102 (*Ancistrocladus likoko derivs*)
Tang, C.-P. *et al., J. Nat. Prod.*, 2000, **63**, 1384-1387 (*Ancistrotectoriline A*)
Bringmann, G. *et al., J. Nat. Prod.*, 2000, **63**, 1465-1470; 2003, **66**, 1159-1165 (*Ancistroealaines A-B, Ancistrotanzanine B, Ancistrotectoriline A*)
Bringmann, G. *et al., Phytochemistry*, 2003, **62**, 631-636; 2008, **69**, 1065-1075 (*Ancistrolikokine D, 6-Demethylancistroealaine, 5′,6-Didemethylancistroealaine, 5-Epiancistrobertsonines*)
Bringmann, G. *et al., Tetrahedron*, 2004, **60**, 4349-4360 (*Ancistroealaine A, Ancistrotanzanine B, synth*)
Bringmann, G. *et al., Tetrahedron*, 2008, **64**, 5563-5568 (*5-Epidemethylancistrobertsonine C, synth*)

Ancistrobrevine C A-981

7-(4,5-Dimethoxy-2-methyl-1-naphthalenyl)-3,4-dihydro-6-methoxy-1,3-dimethyl-8-isoquinolinol
[151870-96-1]



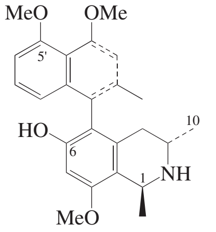
$C_{25}H_{27}NO_4$ 405.493
Alkaloid from stem bark and roots of *Ancistrocladus abbreviatus* (Ancistrocladaceae). Amorph. yellow solid. Mp 180-183°. $[\alpha]_D^{25}$ +13 (c, 0.69 in $CHCl_3$).

1,2-Dihydro, stereoisomer: ***Ancistine***
[58738-33-3]
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from the roots of *Ancistrocladus ealaensis* (Ancistrocladaceae). Cryst. (Me_2CO). Mp 275-276°. $[\alpha]_D^{20}$ -34 (c, 1 in $CHCl_3$/MeOH 1:1). Stereochem. not determined.

Foucher, J.P. *et al., Phytochemistry*, 1975, **14**, 2699 (*Ancistine*)
Bringmann, G. *et al., Phytochemistry*, 1993, **33**, 1511 (*Ancistrobrevine C*)

Ancistrocladine A-982

5-(4,5-Dimethoxy-2-methyl-1-naphthalenyl)-1,2,3,4-tetrahydro-8-methoxy-1,3-dimethyl-6-isoquinolinol, 9CI
[32221-59-3]



Absolute Configuration

$C_{25}H_{29}NO_4$ 407.508
Alkaloid from *Ancistrocladus heyneanus*, *Ancistrocladus congolensis*, *Ancistrocladus hamatus* and *Ancistrocladus tectorius.* Shows antimalarial activity. Cryst. (MeOH). Mp 265-267° dec.

Hydrochloride:
Needles (MeOH/Me_2CO). Mp 220-224° dec. $[\alpha]_D^{25}$ -25.5 (c, 2.3 in MeOH).

N*-Ac:*
Cryst. (Et_2O). Mp 277-279°.

Me ether: ***O-Methylancistrocladine***
[32215-20-6]
$C_{26}H_{31}NO_4$ 421.535
Alkaloid from the root and stem bark of *Ancistrocladus congolensis* (Ancistrocladaceae). Fluffy needles (MeOH). Mp 200-202°.

Me ether; hydrochloride:
Needles (Me_2CO). Mp 315-317° dec. $[\alpha]_D^{25}$ -56.1 (c, 1.9 in $CHCl_3$).

O,N*-Di-Me:* ***O,N-Dimethylancistrocladine***
[32215-13-7]
Alkaloid from the leaves of *Ancistrocladus tanzaniensis.* Prisms (Et_2O). Mp 183-185° (163° dec.). $[\alpha]_D^{25}$ -21 (c, 2.55 in $CHCl_3$).

*4′-*O*-De-Me:* ***4′-O-Demethylancistrocladine***
[165816-69-3]
$C_{24}H_{27}NO_4$ 393.482
Alkaloid from bark of *Ancistrocladus tectorius* (Ancistrocladaceae). Gum. $[\alpha]_D$ +2.5 (c, 1 in $CHCl_3$).

*4′-*O*-De-Me, 6-Me ether:* ***4′-O-Demethyl-6-O-methylancistrocladine***
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from *Ancistrocladus tectorius.* Light yellow powder. $[\alpha]_D^{25}$ -3.1 (c, 0.38 in MeOH).

1,2-Didehydro: ***Ancistrocladinine***
[36209-87-7]
$C_{25}H_{27}NO_4$ 405.493
Minor alkaloid from the roots of *Ancistrocladus heyneanus* (Ancistrocladaceae). Mp 235-238° dec. $[\alpha]_D^{25}$ -321.8 (c, 1.06 in Py).

1,2-Didehydro, Me ether: ***6-O-Methylancistrocladinine***
[134984-06-8]
$C_{26}H_{29}NO_4$ 419.519
Alkaloid from the leaves of *Ancistrocladus tanzaniensis.* Amorph. solid. Mp 102°. $[\alpha]_D^{25}$ -31 (c, 0.4 in MeOH). λ_{max} 231 (log ε 0.22); 303 (log ε 0.04) (MeOH).

1,2,3,4-Tetradehydro: ***Ancistrocladeine***
[58738-34-4]
$C_{25}H_{25}NO_4$ 403.477
Alkaloid from roots of *Ancistrocladus ealaensis* and *Ancistrocladus tectorius* (Ancistrocladaceae). Cryst. (Me_2CO). Mp 275-277°.

1-Epimer: ***Isoancistrocladine****. 1-Epiancistrocladine*
[36209-88-8]
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from roots of *Ancistrocladus heyneanus* (Ancistrocladaceae). Cryst. (MeOH). Mp 230-232°. $[\alpha]_D$ +59.5 (c, 0.6 in $CHCl_3$).

1-Epimer, N*-Me:* ***Ancistrocline***
[82189-88-6]
$C_{26}H_{31}NO_4$ 421.535
Alkaloid from *Ancistrocladus tectorius* (Ancistrocladaceae). Mp 223-224°. $[\alpha]_D^{25}$ +59.1 (c, 0.23 in $CHCl_3$).

*1-Epimer, 5′-*O*-de-Me,* N*-Me:* ***5′-O-Demethylancistrocline***
[828935-65-5]
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from the stem bark of *Ancistrocladus benomensis.* Amorph. brown solid (MeOH). Mp 213°. $[\alpha]_D^{25}$ +61.7 (c, 0.01 in MeOH). λ_{max} 203 (log ε 0.35); 227 (log ε 0.42); 307 (log ε 0.07); 319

(log ε 0.06); 335 (log ε 0.05) (MeOH).

1- And/or 3-epimer, Me ether: ***Ancistroealaensine***
[54382-93-3]
$C_{26}H_{31}NO_4$ 421.535
Alkaloid from the roots of *Ancistrocladus ealaensis* (Ancistrocladaceae). Mp 84° (softens). $[\alpha]_D^{20}$ -26 (c, 1 in MeOH). Config. unknown.

1- And/or 3-epimer, Me ether, perchlorate:
Cryst. (MeOH). Mp 132-135°. $[\alpha]_D^{20}$ -84 (c, 1 in MeOH).

Atropisomer: ***Hamatine***
[56688-90-5]
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from the roots of *Ancistrocladus hamatus* (Ancistrocladaceae). Mp 250-252°. $[\alpha]_D$ +77.44 ($CHCl_3$) (+68). Has opposite chirality of the biaryl system.

Atropisomer, Me ether:
Cryst. (hexane). Mp 160-162°. $[\alpha]_D$ +27.2 (c, 1 in $CHCl_3$).

Atropisomer, O,N*-di-Me:*
Needles (Et_2O). Mp 170-172°.

*Atropisomer, 4′-*O*-de-Me, 6-Me ether:* **4′-O-*Demethyl-6-*O*-methylhamatine***
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from *Ancistrocladus tectorius*. Light yellow powder. $[\alpha]_D^{25}$ +12.4 (c, 0.36 in MeOH).

*Atropisomer, 5′-*O*-de-Me:* **5′-O-*Demethylhamatine***
$C_{24}H_{27}NO_4$ 393.482
Alkaloid from a Congolese *Ancistrocladus* sp. Amorph. solid. Mp 174-180°. $[\alpha]_D^{25}$ +26 (c, 0.1 in MeOH). λ_{max} 237 (log ε 1.42); 309 (log ε 0.41); 322 (log ε 0.37); 337 (log ε 0.34) (CH_2Cl_2).

Atropisomer, 1,2-didehydro: ***Hamatinine***
[194811-19-3]
$C_{25}H_{27}NO_4$ 405.493
Alkaloid from leaves of *Ancistrocladus cochinchinensis*. Isol. as a *ca.* 1:1 inseparable mixt. with Ancistrocladinine.

Atropisomer, 1,2-didehydro, Me ether: **6-O-*Methylhamatinine***
[194242-88-1]
$C_{26}H_{29}NO_4$ 419.519
Alkaloid from leaves of *Ancistrocladus cochinchinensis*. Amorph. $[\alpha]_D^{22}$ +34.1 (c, 1.0 in $CHCl_3$).

*Atropisomer, 1,2-didehydro, 5′-*O*-de-Me:* **5′-O-*Demethylhamatinine***
$C_{24}H_{25}NO_4$ 391.466
Alkaloid from a Congolese *Ancistrocladus* sp. Amorph. yellow solid. $[\alpha]_D^{25}$ +25 (c, 0.1 in MeOH). λ_{max} 235 (log ε 1.05); 311 (log ε 0.34); 321 (log ε 0.33); 335 (log ε 0.3) (CH_2Cl_2).

Atropisomer, 1,2,3,4-tetradehydro, 6-Me ether: **6-O-*Methylhamateine***
$C_{26}H_{27}NO_4$ 417.504
Alkaloid from the leaves of *Ancistrocladus cochinchinensis*. Cryst. ($CHCl_3$/hexane). Mp 233-236°. $[\alpha]_D^{22}$ -41.4 (c, 0.46 in $CHCl_3$).

*Atropisomer, 10-hydroxy, 1,2,3,4-tetradehydro, 4′-*O*-de-Me:* **6-O-*Demethylancistrobenomine A***
[828935-64-4]
$C_{24}H_{23}NO_5$ 405.449
Alkaloid from the stem bark of *Ancistrocladus benomensis*. Pale yellow solid (MeOH). Mp 169°. $[\alpha]_D^{25}$ -34.4 (c, 0.05 in MeOH). λ_{max} 231 (log ε 0.44); 259 (log ε 0.28); 307 (log ε 0.07); 335 (log ε 0.08); 363 (log ε 0.05) (MeOH).

*Atropisomer, 10-hydroxy, 1,2,3,4-tetradehydro, 4′-*O*-de-Me, 6-Me ether:* ***Ancistrobenomine A***
[828935-63-3]
$C_{25}H_{25}NO_5$ 419.476
Alkaloid from the stem bark of *Ancistrocladus benomensis*. Pale yellow powder (MeOH). Mp 270° dec. $[\alpha]_D^{25}$ -21 (c, 0.1 in MeOH). λ_{max} 219 (log ε 1.79); 235 (log ε 2.09); 259 (log ε 1.95); 307 (log ε 0.85); 323 (log ε 0.81); 335 (log ε 0.85); 363 (log ε 0.58) (MeOH).

Atropisomer, 1-epimer, Me ether: ***Ancistrobertsonine B***
$C_{26}H_{31}NO_4$ 421.535
Alkaloid from *Ancistrocladus robertsoniorum*. Mp 192-193°. $[\alpha]_D^{25}$ +4 (c, 0.09 in $CHCl_3$).

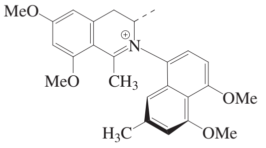
Stereoisomer, O,N*-di-Me: 5-(4,5-Dimethoxy-2-methyl-1-naphthalenyl)-1,2,3,4-tetrahydro-6,8-dimethoxy-1,2,3-trimethylisoquinoline.* ***Ancistrocladonine***
[54382-91-1]
$C_{27}H_{33}NO_4$ 435.562
Alkaloid from the roots of *Ancistrocladus ealaensis* (Ancistrocladaceae). Needles (Et_2O). Mp 82-83°. $[\alpha]_D^{20}$ +20 (c, 1 in MeOH). Stereochem. unknown.

Stereoisomer, O,N*-di-Me, perchlorate:*
Cryst. (MeOH). Mp 256-258°. $[\alpha]_D^{20}$ +71 (c, 1 in MeOH).

Govindachari, T.R. *et al., Tetrahedron*, 1971, **27**, 1013 (*isol, uv, ir, pmr, struct*)
Govindachari, T.R. *et al., J.C.S. Perkin 1*, 1974, 1413 (*config, cryst struct, pmr*)
Foucher, J.P. *et al., Phytochemistry*, 1974, **13**, 1253; 1975, **14**, 2699 (*Ancistrocladine, Ancistroealaensine, Ancistrocladonine*)
Govindachari, T.R. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 871 (*Hamatine*)
Bringmann, G. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 200; 1986, **25**, 913 (*synth, biosynth*)
Bringmann, G. *et al., Heterocycles*, 1989, **28**, 137 (*synth*)
Rizzacasa, M.A. *et al., J.C.S. Perkin 1*, 1991, 2773 (*synth, Ancistrocladinine*)
Bringmann, G. *et al., Phytochemistry*, 1992, **31**, 3297; 1994, **35**, 259; 1999, **52**, 321-332 (*Ancistrocline, Isoancistrocladine, Ancistrorobertsonine B*)
Bringmann, G. *et al., Tetrahedron*, 1993, **49**, 3305 (*cd*)
Fleischhauer, J. *et al., Z. Naturforsch., B*, 1993, **48**, 140 (*cd, Ancistrocladine*)
Montagnac, A. *et al., Phytochemistry*, 1995, **39**, 701 (*4′-O-Demethylancistrocladine*)
Anh, N.H. *et al., Phytochemistry*, 1997, **45**, 1287 (*Hamatinine, O-Methylhamatinine*)
Fleischhauer, J. *et al., Z. Naturforsch., A*, 1998, **53**, 993-996 (*Isoancistrocladine, abs config*)
Tang, C.-P. *et al., J. Nat. Prod.*, 2000, **63**, 1384-1387 (*4′-Demethyl-6-methylancistrocladine, 4′-Demethyl-6-methylhamatine*)
Bringmann, G. *et al., J. Nat. Prod.*, 2004, **67**, 743-748; 2058-2062 (*O,N-Dimethylancistrocladine, 6-O-Methylancistrocladinine, Ancistrobenomine A, 5′-O-Demethylancistrocline*)
Bringmann, G. *et al., Phytochemistry*, 2008, **69**, 1065-1075 (*5′-Demethylhamatine, 5′-Demethylhamatinine*)

Ancistrocladinium A A-983

[918875-18-0]



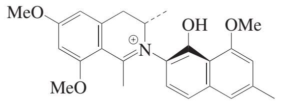
Absolute Configuration

$C_{26}H_{30}NO_4^{\oplus}$ 420.527
Alkaloid from the leaves of *Ancistrocladus* sp. Pale yellow cryst. Mp > 230° dec. $[\alpha]_D^{20}$ -6 (c, 0.05 in MeOH). λ_{max} 214 (log ε 2.73); 225 (log ε 2.69); 335 (log ε 1.65) (MeOH).

Bringmann, G. *et al., J.O.C.*, 2006, **71**, 9348-9356 (*isol, cd, pmr, cmr*)

Ancistrocladinium B A-984

[918875-19-1]
[918875-20-4]



(*R*)*-form*

$C_{25}H_{28}NO_4^{\oplus}$ 406.501
Alkaloid from the leaves of *Ancistrocladus* sp. Pale yellow cryst. Mp > 230° dec. $[\alpha]_D^{20}$ -8 (c, 0.06 in MeOH). Occurs as a mixt. of the two atropisomers, to which the data refers. λ_{max} 227 (log ε 0.94); 346 (log ε 0.34) (MeOH).

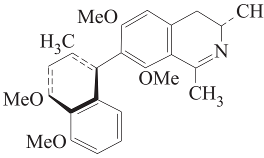
(*R*)*-form*
$[\alpha]_D$ -4.5 (c, 0.04 in MeOH).

(*S*)*-form*
$[\alpha]_D^{20}$ -11.3 (c, 0.04 in MeOH).

Bringmann, G. *et al., J.O.C.*, 2006, **71**, 9348-9356 (*isol, cd, pmr, cmr*)

Ancistrocladisine A-985

7-(4,5-Dimethoxy-2-methyl-1-naphthalenyl)-3,4-dihydro-6,8-dimethoxy-1,3-dimethylisoquinoline, 9CI
[41787-65-9]



Absolute configuration

$C_{26}H_{29}NO_4$ 419.519
Alkaloid from the roots of *Ancistrocladus heyneanus* and *Ancistrocladus hamatus* (Ancistrocladaceae). Pale-brown needles (Et_2O or petrol). Mp 178-180°. $[\alpha]_D^{25}$ +7.8 (c, 0.53 in $CHCl_3$) (synthetic).

Hydrochloride:
Needles (MeOH/Me_2CO). Mp 220-222° dec. $[\alpha]_D$ -16.13 (c, 1.29 in $CHCl_3$).

Methiodide:
Pale-yellow needles. Mp 220-224° dec.

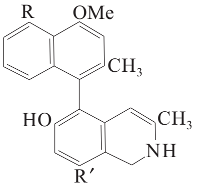
O^6*-De-Me:* ***1,2-Didehydroancistrobertsonine D.*** 6-O-Demethylancistrocladisine

[250131-08-9]
$C_{25}H_{27}NO_4$ 405.493
Alkaloid from *Ancistrocladus robertsoniorum*. Cryst. (MeOH aq.). Mp 185-187°. $[\alpha]_D^{25}$ -30 (c, 0.04 in $CHCl_3$).

Govindachari, T.R. *et al., Indian J. Chem.*, 1972, **10**, 1117 (*uv, pmr, isol, struct*)
Govindachari, T.R. *et al., J.C.S. Perkin 1*, 1975, 2134 (*uv, abs config*)
Parthasarathy, P.C. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 590 (*cryst struct*)
Bringmann, G. *et al., Angew. Chem., Int. Ed.*, 1989, **28**, 1672 (*synth*)
Bringmann, G. *et al., Phytochemistry*, 1999, **52**, 321-332 (*1,2-Didehydroancistrorobertsonine D*)

Ancistrocongine A-986

1,2-Dihydro-5-(4-methoxy-2-methyl-1-naphthalenyl)-3-methyl-6,8-isoquinolinediol, 9CI
[56973-82-1]



R = H, R′ = OH

$C_{22}H_{21}NO_3$ 347.413
Alkaloid from the roots of *Ancistrocladus congolensis* (Ancistrocladaceae). Cryst. (Me_2CO). Mp 298-299°. $[\alpha]_D$ 0 (MeOH).

Foucher, J.P. *et al., Plant. Med. Phytother.*, 1975, **9**, 87 (*isol, spectra, struct*)

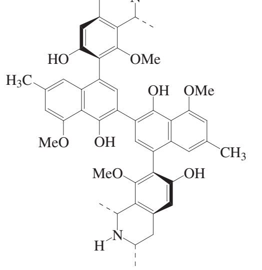
Ancistrocongolensine A-987

5-(4,5-Dimethoxy-2-methyl-1-naphthalenyl)-1,2-dihydro-8-methoxy-3-methyl-6-isoquinolinol, 9CI
[56973-81-0]
As Ancistrocongine, A-986 with R = R′ = OMe
$C_{24}H_{25}NO_4$ 391.466
Alkaloid from the roots of *Ancistrocladus congolensis* (Ancistrocladaceae). Cryst. (Me_2CO). Mp 258°. $[\alpha]_D$ 0 (MeOH).

Foucher, J.P. *et al., Plant. Med. Phytother.*, 1975, **9**, 87 (*isol, spectra, struct*)

Ancistrogriffithine A A-988

[346702-11-2]



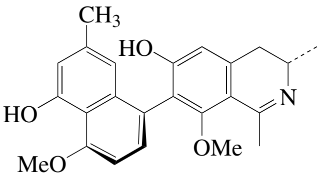
Absolute Configuration

$C_{48}H_{52}N_2O_8$ 784.947
Alkaloid from *Ancistrocladus griffithii*. Light yellow powder (MeOH). Mp 230° dec. $[\alpha]_D^{25}$ +73.5 (c, 0.3 in MeOH).

Bringmann, G. *et al., Phytochemistry*, 2002, **61**, 195-204 (*isol, pmr, cmr, ms, cd*)

Ancistroheynine A A-989

[185417-34-9]



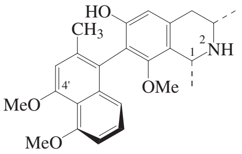
Absolute Configuration

$C_{24}H_{25}NO_4$ 391.466
Alkaloid from *Ancistrocladus heyneanus*. Antimalarial agent. Yellow amorph. powder. $[\alpha]_D^{25}$ +68 (c, 0.3 in $CHCl_3$).

Bringmann, G. *et al., Phytochemistry*, 1996, **43**, 1405 (*isol, ir, pmr, cms, ms, cd, struct*)

Ancistrorobertsonine D A-990

[250131-22-7]



Absolute Configuration

$C_{25}H_{29}NO_4$ 407.508
Alkaloid from *Ancistrocladus robertsoniorum*. Amorph. yellow powder. Mp 133-134°. $[\alpha]_D^{25}$ +82 (c, 0.51 in $CHCl_3$).

N-*Me*: ***6-O-Demethyl-8-O-methyl-7-epiancistrobrevine D***. N-*Methylancistrorobertsonine D*
[169168-91-6]
$C_{26}H_{31}NO_4$ 421.535
Alkaloid from the leaves of *Ancistrocladus cochinchinensis*.

*8-*O*-De-Me,* N*-Me:* ***6-O-Demethyl-7-epiancistrobrevine D***
[194141-89-4]
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from the leaves of *Ancistrocladus cochinchinensis*. Cryst. ($CHCl_3$/hexane). Mp 229-232°. $[\alpha]_D^{22}$ +51.8 (c, 0.49 in $CHCl_3$).

*8-*O*-De-Me,* O^6,N*-di-Me:* ***7-Epiancistrobrevine D***
[194242-89-2]
$C_{26}H_{31}NO_4$ 421.535
Alkaloid from the leaves of *Ancistrocladus cochinchinensis*. Cryst. ($CHCl_3$/hexane). Mp 177-178°. $[\alpha]_D^{22}$ +46.1 (c, 1 in $CHCl_3$).

*1-Epimer, 4′-*O*-de-Me, 6-Me ether:* ***Ancistrotectoriline B***
[302543-64-2]
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from *Ancistrocladus tectorius*. Light yellow powder. $[\alpha]_D^{25}$ +79.1 (c, 0.46 in $CHCl_3$).

*1-Epimer, 8-*O*-de-Me:* ***Ancistrogriffine B***
[478796-15-5]
$C_{24}H_{27}NO_4$ 393.482
Alkaloid from *Ancistrocladus griffithii*.

3-Epimer: ***Ancistrocongoline D***
[455255-22-8]
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from the root bark of *Ancistrocladus congolensis*. Brownish powder. Mp 232°. $[\alpha]_D^{24}$ -6.7 (c, 0.52 in $CHCl_3$).

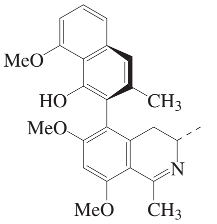
Stereoisomer: 7-(4,5-Dimethoxy-2-methyl-1-naphthalenyl)-1,2,3,4-tetrahydro-8-methoxy-1,3-dimethyl-6-isoquinolinol. ***Ancistrine***
[58738-35-5]
$C_{25}H_{29}NO_4$ 407.508
Alkaloid from the roots of *Ancistrocladus ealaensis*. Cryst. (Me_2CO). Mp 230-231°. $[\alpha]_{Hg}^{20}$ -35 (c, 1 in MeOH). Stereochem. not determined-identity uncertain.

*Atropisomer, 8-*O*-de-Me,* O^6,N*-di-Me:* ***Ancistrobrevine D***
[167503-63-1]
$C_{26}H_{31}NO_4$ 421.535
Alkaloid from *Ancistrocladus abbreviatus*. Mp 172°. $[\alpha]_D^{25}$ +24.9 (c, 0.37 in $CHCl_3$).

Foucher, J.P. *et al., Phytochemistry*, 1975, **14**, 2699-2702 (*Ancistrine*)
Bringmann, G. *et al., Planta Med.*, Suppl.1, 1992, **58**, 703-704 (*Ancistrobrevine D*)
Anh, N.H. *et al., Phytochemistry*, 1997, **45**, 1287-1291 (*7-Epiancistrobrevine D derivs*)
Bringmann, G. *et al., Phytochemistry*, 1999, **52**, 321-332 (*isol, cd, ir, pmr, cmr, ms, abs config*)
Tang, C.-P. *et al., J. Nat. Prod.*, 2000, **63**, 1384-1387 (*Ancistrotectoriline B*)
Bringmann, G. *et al., J. Nat. Prod.*, 2002, **65**, 1096-1101 (*Ancistrocongoline D*)
Bringmann, G. *et al., Phytochemistry*, 2002, **61**, 195-204 (*Ancistrogriffine B*)

Ancistrotanzanine A A-991

[613245-54-8]



Absolute Configuration

$C_{25}H_{27}NO_4$ 405.493
Alkaloid from *Ancistrocladus tanzanien-*